CASE Department

Group Leader: ARNAU FOLCH (In collaboration with Senior Research Engineer ALEXANDRE MARTI)

https://www.bsc.es/discover-bsc/organisation/scientific-structure/environmental-simulations

Research project/ Research Group description

Project 1:

The fellow will join the Environmental Simulations (ES) group at the CASE Department, to develop satellite---supported procedures and algorithms to rapidly determine the distribution of ash in the air and compare it with the outcome of the BSC VADT model forecasts. The candidate will employ these procedures to establishing an operational validation protocol for forecast---based volcanic ash products. The protocol should:

- Quantify and understand the spatial and temporal variation in the skill of volcanic ash simulations when compared to satellite observations.
- Assess the behavior of data assimilation methods.
- Quantify the sensitivity of forecast skill to changes in model formulation.
- Collaborate with researchers in charge of the CASE Atmospheric Impact Services to develop measures for air traffic management to improve the ability to react in the case of future volcanic eruptions.

After the first year, the fellow will spend a 3---months secondment in a BSC spin---off (Mitiga Solutions) to provide credible scientific expertise to improve risk management across multiple industries following the international regulations established by International Civil Aviation Organization (ICAO). The results of this research stay will be presented in the framework of the Severo Ochoa research seminars.

Thorough the fellowship, the candidate is expected to receive a combination of training from the BSC's Education and Training Unit, the Centre's HR service and the scientific departments. The Environmental Simulations group at CASE will provide training for the BSC's VADT (HPC) models to forecast atmospheric natural hazards. Dr. A. Folch and Dr. A. Marti will facilitate the fellow's integration into the BSC.

CASE Department

Group Leader: ARNAU FOLCH

https://www.bsc.es/discover-bsc/organisation/scientific-structure/environmental-simulations

Research project/ Research Group description

Project 2:

The fellow will join the Environmental Simulations (ES) group at the CASE Department, with research lines on mesoscale and microscale meteorological modelling, wind energy, and atmospheric transport modelling. He/she will perform research on explicit Large Eddy Simulations (LES) atmospheric model implementations using the in-house multiphysics Alya solver on both general purpose and emerging hardware architectures towards Exascale computing (e.g. FPGAs). Research applications will focus on the fields of wind energy (modelling of on-shore and off-shore wind farms considering all aspects affecting surface layer atmospheric flows in complex terrains) and high-resolution wind field modelling and dispersion of pollutants at urban-scale. The wind energy application will be done in collaboration with a world leading industry (Iberdrola Renovables) through the SEDAR ("Simulación eólica de alta resolución") project. In addition, the fellow will also collaborate giving a transversal service to the following on-going projects:

• GrowSmarter (www.grow-smarter.eu) in developing a modelling strategy to monitor urban air quality parameters through numerical simulations considering the city of Barcelona as a test case.

• LegaTo in improving the Alya LES-CFD explicit solver efficiency in a demonstrator for future operational air quality modelling system based on CFD and covering large urban domains at high resolution (tens of meters).

• Energy oriented Center of Excellence for computer applications (EoCoE, www.eocoe.eu) in modelling wind in complex terrains accounting for wind turbine rotor and wake effects.

CASE Department

Group Leader: MERVI MANTSINEN

http://fusion.bsc.es/

Research project/ Research Group description

Project 3:

In the Fusion group (fusion.bsc.es) at the Department of Computer Applications in Science and Engineering (CASE), the fellow will carry out a research project of his / her choice focused on numerical modelling of experiments in magnetically confined fusion devices in preparation for ITER operation (www.iter.org), working towards the objectives of the European fusion research programme in collaboration with ITER, the International Tokamak Physics Activity (https://www.iter.org/org/team/fst/itpa), EUROfusion and the Spanish national fusion laboratory CIEMAT. EUROfusion (www.euro-fusion.org) is the "European Consortium for the Development of Fusion Energy" which manages and funds European fusion research activities on behalf of Euratom. His / her research project will be well aligned to the overall objective of the group, which is to enhance the modelling capabilities in fusion by code development, validation, integration and optimization including the use of advanced High Performance Computing (HPC) techniques, with the ultimate goal of helping improve the performance of ITER and future fusion reactors. In order to improve physics understanding and validate physical and numerical models, the fellow will join the group's existing collaborations on experiments on present devices such as the Joint European Torus (JET), which is the world largest operating fusion device located near Oxford (UK).

The research topic can be within the present research lines of the group, or it could be a new topic that fits the above overall objective of the group. The present main research lines of the group are

- Plasma heating by electromagnetic waves in the ion cyclotron range of frequencies (ICRH)
- Production and behaviour of fast ions in fusion plasmas
- Non-Linear MHD modelling to study mitigation of Edge Localized Modes (ELMs) by pellet injection
- HPC for multi-physics modelling of fusion reactor components
- Fusion materials modelling

Regarding training, the Fusion group is dedicated to providing high-quality postdoctoral training for the fellow. It draws upon its experience in developing specific technical and scientific skills, as well as the complementary skills required for efficient research execution and communication. The fellow work with human resources, education department and the supervisor to develop and execute an individual Career Plan, which draws upon the experience of the BSC and the needs of the researcher. The training objectives in the plan are monitored and updated regularly in meetings undertaken with the supervisor, discussing research progress

and identifying potential difficulties and ways of overcoming them. Specific training actions are courses on high performance computing, plasma physics and controlled fusion, fusion technology and professional growth. The courses are chosen based on the training needs and interests of the fellow.

CASE Department

Group Leader: JOSE IGNACIO LATORRE SENTIS (In collaboration with Senior Researcher POL FORN)

https://www.bsc.es/research-and-development/research-areas/quantum-information

Research project/ Research Group description

Project 4:

The QUANTIC group at BSC consists in two interrelated teams: quantum algorithms and superconducting quantum processors. The applicant to the STARS programme will have the chance to choose which of the two teams s/he will join. Under the quantum algorithms group, led by Prof. Latorre, the research will focus on developing novel quantum algorithms for small-scaled quantum processors performing quantum gates, quantum simulation and quantum annealing. The fellow will receive training in quantum algorithms and machine learning and in using the supercomputer MareNostrum in order to study the limits of classical computation and the regime where a quantum computer provides a quantum speedup. In the superconducting quantum processors team, led by Dr. Forn-Díaz, the fellow will join an experimental team to manufacture and measure superconducting circuits and operate them to perform quantum computing applications. The team is working towards quantum annealing applications using qubits with coherence, and in this way explore the quantum speedup over classical computation and other existing prototypes of quantum processors. The fellow will receive training in nanolithography, cryogenics, microwave engineering and experience operating a quantum processor.

CASE Department

Group Leader: JOSEP DE LA PUENTE

https://www.bsc.es/research-development/research-areas/geophysics/hpc-geophysical-applications

Research project/ Research Group description

Project 5:

The candidate will be involved in research related to the imaging of the Earth's interior by means of geophysical methods and the study of the physical nature and societal impact of earthquakes. In particular, the group develops 3D modelling and inversion algortithms for seismic and electromagnetic waves using HPC hardware to a maximum efficiency. Similarly, other R&D efforts are related to modelling earthquake scenarios and evaluating the consequences of such events in realistic conditions. Last but not least we have an interest on tackling very high dimensional models (i.e. parametric models), uncertainty quantification and machine learning applied to geophysics from an HPC point of view.

CASE Department & Computer Sciences Department

Group Leader: GUILLAUME HOUZEAUX (In collaboration with Researcher MARTA GARCIA GASULLA)

https://www.bsc.es/discover-bsc/organisation/scientific-structure/physical-and-numerical-modelling

Research project/ Research Group description

Project 6:

Computer Applications in Science and Engineering (CASE) department is developing the High Performance Computational Mechanics code Alya, a multi-physics simulation code to solve large and complex coupled problems in different fields of engineering: biomechanics (cardiovascular & respiratory systems), aeronautics (structures, aerodynamics), energy (fusion, wind). Among other activities, the Computer Science (CS) department develops methodologies and tools to boost the efficiency of simulation codes on current and prototype architectures. This project aims at enabling and optimizing Alya for exascale architectures, through a collaboration between CASE and CS departments.

The fellow will explore all the levels of parallelism offered by modern architectures, at the node, chip and superscalar core/accelerator levels. This will require to work with different parallel programming languages and paradigms, like MPI, OpenMP, languages or pragmas (CUDA, OpenCL, OpenACC) for accelerators (GPU, FPGA), but also to manage the different tools developed at CS. Specially, the performance analysis tools (i.e. Extrae and Paraver) and the different runtime libraries (i.e. DLB or Nanos++ RTL).

The fellow will be integrated in the CASE department, where a wide range of applications is treated, all with specific computational requirements. Teamwork will thus be a must in order to collaborate not only with the different application teams but also with the researchers from the CS department.

Computer Sciences Department

Group Leader: ANTONIO PEÑA

https://www.bsc.es/discover-bsc/organisation/scientific-structure/accelerators-and-communications-hpc

Research project/ Research Group description

Project 7:

The Accelerators and Communications for HPC team leads cutting-edge research and development around accelerators/coprocessors in HPC. We collaborate closely with the two major accelerator/coprocessor vendors for HPC: NVIDIA and Intel. While we run the BSC/UPC NVIDIA GPU Center of Excellence, we also collaborate with the Intel-BSC Exascale Lab. activities. We organize locally international events such as the PUMPS Summer School, PATC Courses on CUDA/OpenACC, and the Annual BCS/UPC HPC Hackathon, and collaborate in the organization of related international conferences and workshops such as SC, HiPC, SCALE, AsHES, WACCPD, and ROME. We are also involved in low-level networking and MPI research.
Our broad mission is driving top-notch research and development around accelerators and communications technology for HPC. This can be framed in three main points:

Helping vendors advance their hardware architecture and software stack.
Designing and developing programming models, runtime systems, and libraries supporting accelerated computing and networking.
Developing and porting coprocessor-accelerated and distributed-memory applications.

The successful candidate will become the technical lead of one of our research lines, according to his/her background, and will be involved in one secondary project, while assisting on the several research tasks of the team (developing papers, writing proposals, etc.). There are also possibilities to get involved in organization committees of international events and mentoring junior members/visitors.

Computer Sciences Department

Group Leader: ROSA M BADIA

https://www.bsc.es/discover-bsc/organisation/scientific-structure/workflows-and-distributed-computing

Research project/ Research Group description

Project 8:

This fellow will perform research to address the limitations of current large scale data processing tools by proposing a scalable and highly programmable framework that can be employed in several distributed platforms, including HPC clusters. This research will contribute to the needs of convergence between HPC and Big Data, specially in the area of programming models. The research will be based in COMPSs, a framework designed to allow the development of distributed applications in an effortless manner, that can be employed by researchers and domain experts not familiarized with parallel programming. COMPSs is a task-based programming model developed by the Workflows and Distributed Computing group at BSC, targeting distributed computing platforms. More specifically, the fellow will do research in three areas: Efficient integration of COMPSs with distributed storage systems; implementation of a distributed machine learning library for COMPSs; and support to other researchers in the development of scientific COMPSs applications.

Computer Sciences Department

Group Leader: FRANCISCO CAZORLA

https://www.bsc.es/discover-bsc/organisation/scientific-structure/computer-architecture-operating-systems-caos

Research project/ Research Group description

Project 9:

The CAOS group seeks for excellent candidates to carry out research in the topic of parallel, critical, embedded applications and high-performance hardware architectures for future autonomous vehicles in domains such as automotive, railway, avionic or space. The research activities cover:

- Dealing with real state-of-the art computing boards that can be used in future autonomous vehicles (e.g. cars). This includes the characterization and benchmarking of those platforms in relevant metrics for the critical markets e.g. (worst-case) performance, predictability, reliability, energy and power, as well as addressing the programmability of these devices. The candidates will obtain hands-on experience with the platforms and their corresponding software stacks.
- Making cutting-edge proposals on hardware/software to support the performance needs of future embedded applications. To that end, appropriate simulation and emulation infrastructure(s) will be developed/adapted to permit the modelling of complex existing hardware like the real boards of the previous activity, and will allow the evaluation of the hardware proposals to be devised. On the software side, solutions related to programmability, reliability, timing analysis and certification will be proposed. Therefore, the candidates will receive all the necessary training related to the specific hardware or software solution that they will consider in their research.
- Dealing with parallel applications – based on AI algorithms – for perception (image recognition), fusion and decision making. In this activity, existing code bases will be studied and ported to the aforementioned platforms, in order to study their characteristics, while their performance will be tuned for optimal results. Moreover, new contributions are expected to be made in terms of AI and new relevant applications will be developed. The candidates will get experience in automotive application design and development, as well as on the field of machine learning.

Computer Sciences Department

Group Leader: MIQUEL MORETO and MARC CASAS

https://www.bsc.es/research-development/research-areas/computer-architecture-and-codesign/runtime-aware-architectures

Research project/ Research Group description

Project 10:

High performance architectures for genomics data analytics. The goal of the research team is to design novel high performance and energy-efficient parallel architectures for genomics data analytics. These applications are a critical component in the success of precision medicine: sequencing and analysing the whole genome of a patient will allow anticipating health problems, and promoting personalized and preventive therapies. With the advent of next-generation sequencing, the amount of genomic data available to researchers is increasing exponentially and, in the next decade, hundreds of millions of genomes will need to be analysed every year. At present, genomics data analytics are extremely data-intensive, suffering from inefficient computations on current architectures. As a result, the performance bottleneck in these applications is moving from the sequencing side (as it used to be in the last decade) towards the computing side. Simply relying on new and faster processors will not be enough to address this challenge.

In this context, the research team targets a ground-breaking approach to improve the performance and energy efficiency of genomics data analytics by completely redesigning the underlying parallel architecture. In data-intensive applications, the energy cost of data transfer is greater than that required for floating point operations. This paradigm shift motivates the research team to design data-centric architectures, novel system architectures that bring processing capabilities closer to the data. Also, novel accelerators and enhanced vector functionalities for genomics data analytics will be explored, achieving a tight integration of these accelerators and the data-centric architecture. Finally, a co-design cycle between the architecture and genomics applications will be developed in order to design energy-efficient architectures for faster and more effective data analysis. As a result of this research, precision medicine based on genomics analysis may become a plausible reality for European citizens in the next decade.

Computer Sciences Department

Group Leader: JOSEP CASANOVAS

https://www.bsc.es/discover-bsc/organisation/scientific-structure/hpc-modelling-and-simulation-social-sciences

Research project/ Research Group description

Project 11:

The HPC Modeling and Simulation for Social Sciences research group at BSC-CNS works on applying novel quantitative methods to explore human behavior using an evolutionary framework. Therefore, their research is multidisciplinary, combining mathematical modelling techniques from statistics and operations research with applications in social sciences (anthropology, demography and archaeology mainly), in biomedicine (epidemics) and fostering the use of High Performance Computing (HPC) to run large-scale models in size and complexity. Techniques such as Agent-Based Models and spatio-temporal analysis to explore the emergence of social interaction are often used in the performed research. The research lines of work for a candidate will be any of the following:

1. Explore the implications of these methodologies to the spread of diseases in the context of epidemic dispersal, offering solution to epidemiological emergencies, and proposing ways out to ageing.
2. Evaluate the impact of our developed tools in providing assistance in the territory management policies, both in the context of resilient (smart) cities and in slowing down the progressive abandon of rural areas to urban.
3. Research in Robotic Innovation in Urban Areas to face the urban challenges proposed by European cities to offer novel robotics solutions addressed to public demand.
4. Research and apply HPC technologies to offer competitive solutions to users to enhance the performance of the social agent-based simulation platform.

The main goal of the candidate's work would be to explore new methodologies to foster the use of HPC methodologies in the understanding and forecasting of human social dynamics related to ageing, territorial balance or disease transmission. The candidate would be involved in current projects related to these subjects and would receive the training from specialist in different areas such as computer science, physics engineering, medicine, anthropology and history.

Computer Sciences Department

Group Leader: FILIPPO MANTOVANI

https://www.bsc.es/research-development/research-areas/computer-architecture-and-codesign/mobile-and-embedded-based-hpc

Research project/ Research Group description

Project 12:

Deploy state-of-the-art data analytics technologies in an industrial environment leveraging advanced. HPC techniques and programming models. The fellow will be involved in analysis and visualization of large industrial datasets using both, standard and ad-hoc data analysis tools with the goal of performing on line data analysis of large manufacturing industrial plants and study offline optimization techniques in close interaction with industrial machinery providers.
Analysis and improvement of power monitoring tools and energy consumption in an HPC environment. Using the Mont-Blanc platforms and BSC tools the fellow will be involved in activities such as static and dynamic frequency scaling of large scientific applications with the possibility of implementing ideas for reducing "energy to solution" on state-of-the-art HPC computational platforms.

Computer Sciences Department

Group Leader: OSMAN UNSAL and ADRIAN CRISTAL

https://www.bsc.es/discover-bsc/organisation/scientific-structure/computer-architecture-parallel-paradigms

Research project/ Research Group description

Project 13:

Low energy DNN based on multiple FPGAs. FPGAs are a very good low energy hardware substrate to implement computational dense applications. Deep Neural Network (DNN) applications are strongly in this category, because they require a large number of multiply-add operations. However, the FPGAs are limited by the number of computational resources that can fit in the chip and also by the amount of memory that they can support in the chip. A large DNN has to be split across many FPGAs. The partitioning can potentially add another problem: communication between the FPGAs. Therefore, smart DNN partitioning heuristics must be developed to fulfill all these constraints. In addition to smart partitioning we will also research how we can reduce the internal FPGA resources via compression and/or reduceed precision. Our idea is to work on both the training and the inference phases of the DNN.

STARS
POST-DOCTORAL PROGRAMME

Barcelona Supercomputing Center
Centro Nacional de Supercomputación
EXCELENCIA SEVERO OCHOA
HR EXCELLENCE IN RESEARCH

Computer Sciences Department

Group Leader: OSMAN UNSAL and ADRIAN CRISTAL (In collaboration with Senior Researcher LEONARDO BAUTISTA and Senior Researcher MARC CASAS)

https://www.bsc.es/discover-bsc/organisation/scientific-structure/computer-architecture-parallel-paradigms

Research project/ Research Group description

Project 14:

One promising idea in algorithms of approximate nature is to employ multi-precision arithmetic to reduce computational costs without significantly compromising the quality of solution. This idea has already been applied at BSC to multi-grid solvers, and is indeed pertinent to other fields like tensor-based approximate techniques.
In a distributed framework, one can also consider reducing the precision of the communication elements in an effort to decrease the volume of communication, and thereby achieve better scalability, with reasonable trade-offs in the quality of solution. We are hoping with this project to better investigate this direction of research on a multi-grid solver as a first step, and also extend these ideas to tensor computations."

European Commission

Computer Sciences Department

Group Leader: OSMAN UNSAL and ADRIAN CRISTAL (In collaboration with Senior Researcher LEONARDO BAUTISTA)

https://www.bsc.es/discover-bsc/organisation/scientific-structure/computer-architecture-parallel-paradigms

Research project/ Research Group description

Project 15:

HPC systems consistently increase in scale and complexity with each successive generation. This is necessary to keep pace with the growing computational demands of ever-increasing problem sizes and precision requirements. Moving data across HPC systems has always been a source of performance bottlenecks, causing data movement challenges to become more prevalent for modern large problem sets, or Big Data workloads. In our previous work we presented a method for undertaking performance analysis of compound communication routines, such as MPI collectives, running on large-scale InfiniBand networks in order to detect the network bottlenecks withing such complex data movement routines. Our work resulted in the development of a lightweight, low-level MPI profiler (called ibprof) and a visualization module to non-intrusively and accurately reflect traffic over the physical topology of the network. Moving forward, we aim to better understand and predict the performance loss due to interference on emerging systems. Specifically, as network resources continue to be shared by inter-node communication traffic and parallel I/O traffic, the network interference caused by emerging I/O architectures must be studied, predicted, and mitigated. Additionally, as node-sharing scheduling policies become more widely deployed in pursuance of increased system utilization, more relevant models are required to guide the efficient co-location of the new Big Data workloads alongside traditional HPC workloads. The results of these studies will benefit, among other things, the development of better job scheduling policies, network routing algorithms, and virtualization strategies.

Earth Sciences Department

Group Leader: FRANCISCO DOBLAS-REYES

https://www.bsc.es/discover-bsc/organisation/scientific-structure/climate-prediction

Research project/ Research Group description

Project 16:

The fellow will work on the development of innovative solutions to produce ensemble global climate predictions for decadal (one to forty years into the future) time scales with both the EC-Earth model and a coordinated multi-model. The research will focus on aspects that characterise uncertainty in climate predictions, the production of action-oriented regional climate information and the evaluation against observations. Methodologies for generating seamless sources of information that merge global initialised and non-initialised simulations will be explored for the first time, addressing the key question of the length of period of overlap and the merging points in time. The simulations will be co-designed with users to constitute a robust foundation for Europe-wide climate service activities to support climate-related risk assessments and climate change adaptation programmes. This should lead to the demonstration of the value of climate predictions through illustrations focusing on high impact extreme weather events.

The researcher will improve his/her coding and data analysis skills via the PATC courses (organized by PRACE, Partnership for Advanced Computing in Europe <www.bsc.es/education/training/patc-cour
ses>) and the regular training of the Computational Earth Sciences group of the department. The latter also focuses on improving scientific and project writing abilities, and will introduced the researcher to project management. All this will be implemented via the formal courses organized by the Education and Training team and Human Resources, and the participation in the regular seminars organized by the department.

The proposed research will be managed through fortnightly meetings with the supervisor to ensure full coherence between the research planned and the general objectives of the department. Regular meetings will take place involving the rest of the department members, especially those in the Climate Prediction and Earth System Services groups, to ensure an adequate integration of this research into the rest of the research carried out in the department. In this context, the applicant will be encouraged to participate in discussions and meetings involving the H2020-funded project EUCP.

Earth Sciences Department

Group Leader: PABLO ORTEGA and LOUIS PHILIPPE CARON

https://www.bsc.es/discover-bsc/organisation/scientific-structure/climate-prediction

Research project/ Research Group description

Project 17:

Research activities for a "Seasonal-to-decadal climate forecaster" research line:

The Climate Prediction group offers to host one or more fellows to work on the development of regional and global climate prediction capabilities and related services for time scales ranging from a few weeks to a few decades into the future (sub-seasonal to decadal climate prediction). The research will involve expanding our understanding of the climate processes that contribute to this prediction, through a combined deep analysis of the state-of-the-art climate forecast systems and the most up-to-date observational datasets. In particular, the envisaged analyses include an investigation of the linkages between both sea-ice and the ocean and the climate of the mid-latitudes, as well as the role of the atmosphere dynamics for prediction in the North Atlantic/European region, with a particular focus on extreme events.

The researcher/s will improve their coding and data analysis skills via the PATC courses (organized by PRACE, Partnership for Advanced Computing in Europe <www.bsc.es/education/training/patc-cour
ses>) and the regular training of the Computational Earth Sciences group of the department. The latter also focuses on improving scientific and project writing abilities, and will introduce the researcher/s to project management. All this will be implemented via the formal courses organized by the Education and Training team and Human Resources, and the participation in the regular seminars organized by the department.
The proposed research will be managed through fortnightly meetings with the supervisor to ensure full coherence between the research planned and the general objectives of the department. Regular meetings will take place involving the rest of the department members, especially those in the Computing Earth Science and Earth System Services groups, to ensure an adequate integration of this research into the rest of the research carried out in the department. In this context, the applicant/s will be encouraged to participate in discussions and meetings involving the H2020-funded projects APPLICATE/PRIMAVERA.

Earth Sciences Department

Group Leader: CARLOS PEREZ GARCIA-PANDO

https://www.bsc.es/discover-bsc/organisation/scientific-structure/atmospheric-composition

Research project/ Research Group description

Project 18:

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 aerosol consists primarily of insoluble Fe that is partly transformed into bioavailable Fe species during atmospheric transport through a variety of dissolution mechanisms, such as 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.
The fellow will work on improving our understanding of the atmospheric delivery of bioavailable Fe to the ocean. He/she will contribute to 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. The 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. The fellow will emphasize on novel aspects such as the role of dust mineralogy and anthropogenic dust sources in the deposition of soluble Fe.

The researcher will improve his/her coding and data analysis skills via the PATC courses (organized by PRACE, Partnership for Advanced Computing in Europe <www.bsc.es/education/training/patc-courses>) and the regular training of the Computational Earth Sciences group of the department. Training activities also focus on improving scientific and project writing abilities, and will introduce the researcher to project management. All this will be implemented via the formal courses organized by the Education and Training team and Human Resources, and the participation in the regular seminars organized by the department. The proposed research will be managed through biweekly meetings with the supervisor to ensure full coherence between the research planned and the general objectives of the department. Regular meetings will take place involving the rest of the department members, especially those in the Atmospheric Composition group, to ensure an adequate integration of

this research into the rest of the research carried out in the department. In this context, the applicant will be encouraged to participate in discussions and meetings involving several funded projects related to the fellow´s work including the AXA Chair on Sand and Dust Storms, an ERC Consolidator Grant entitled FRAGMENT (FRontiers in dust minerAloGical coMposition and its Effects upoN climaTe) and a MINECO grant entitled NUTRIENT (QuaNtifying the present and fUTure atmospheric deliveRy of bIoavailablE iroN to The ocean) led by the Supervisor.

Earth Sciences Department

Group Leader: CARLOS PEREZ GARCIA-PANDO and ORIOL JORBA

https://www.bsc.es/discover-bsc/organisation/scientific-structure/atmospheric-composition

Research project/ Research Group description

Project 19:

The Atmospheric Composition group of the Earth Sciences Department at BSC aims at better understanding and predicting the spatiotemporal variations of atmospheric pollutants along with their effects upon air quality, weather and climate. The AC group develops the Multiscale Online Non-hydrostatic AtmospheRe CHemistry model (MONARCH). MONARCH contains advanced chemistry and aerosol packages, and is coupled online with the Non-hydrostatic Multiscale Model (NMMB), which allows for running either global or high-resolution (convection-allowing) regional simulations, and is coupled with an aerosol data assimilation system based on the Local Ensemble Transform Kalman Filter (LETKF).
The fellow will work on improving our understanding of aerosol-chemistry processes in the atmosphere through numerical experiments with the MONARCH model. New aerosol and chemistry processes will be implemented and tested in the system to improve current forecasting capabilities and advance our understanding of chemistry-weather-climate interactions. The fellow will contribute to enhance the current treatment of some aerosol components in MONARCH (i.e., mineralogical composition of dust aerosol, secondary organic aerosols, brown carbon), introduce new species (i.e., aerobiological aerosol species like birch pollen, grass pollen or olive pollen), and extend the assimilation capabilities of the system considering gas-phase observations. The AC group contributes to a variety of forecasting activities: the dust component of MONARCH runs operationally at the first WMO Regional Specialized Meteorological Center for Atmospheric Sand and Dust Forecast (i.e., the Barcelona Dust Forecast Center, BDFC), and contributes to multi-model ensemble forecasts both at the WMO Sand and Dust Storm Warning Advisory and Assessment System Regional Center (WMO SDS-WAS RC) for Northern Africa, the Middle East and Europe, and the International Cooperative for Aerosol Prediction (ICAP). Both WMO Regional Centers are co-hosted by BSC and the Spanish Meteorological Agency (AEMET). The group also develops and maintains the CALIOPE air quality system ("CALIdad del aire Operacional Para España"), which provides high-resolution air quality forecasts over Europe and Spain using the in-house emission model HERMES. CALIOPE will be based on MONARCH model in the near future and aims to contribute to the Copernicus European air quality ensemble model. The models and forecasts are enhanced by an intensive use of up-to-date observations, both for model evaluation and to feed the aerosol ensemble-based data assimilation system.The researcher will improve his/her coding and data analysis skills via the PATC courses (organized by PRACE, Partnership for Advanced Computing in Europe <www.bsc.es/education/training/patc-courses>) and the regular training of the Computational Earth Sciences group of the department. Training activities also focus on improving scientific and project writing abilities, and will introduce the

researcher to project management. All this will be implemented via the formal courses organized by the Education and Training team and Human Resources, and the participation in the regular seminars organized by the department. The proposed research will be managed through biweekly meetings with the supervisor to ensure full coherence between the research planned and the general objectives of the department. Regular meetings will take place involving the rest of the department members, especially those in the Atmospheric Composition group, to ensure an adequate integration of this research into the rest of the research carried out in the department. In this context, the applicant will be encouraged to participate in discussions and meetings involving several funded projects related to the fellow´s work including the AXA Chair on Sand and Dust Storms and an ERC Consolidator Grant entitled FRAGMENT (FRontiers in dust minerAloGical coMposition and its Effects upoN climaTe) led by the Group Manager of the AC group.

Earth Sciences Department

Group Leader: ALBERT SORET

https://www.bsc.es/discover-bsc/organisation/scientific-structure/earth-system-services

Research project/ Research Group description

Project 20:

The Earth System Services Group (ESS; www.bsc.es/ess) seeks a climate scientist with interest in climate services to work in both renewable energy and agriculture sectors. ESS aims at developing tailored services on weather and atmospheric composition model simulations (focussing on short-term time scales) and climate predictions (focusing on the sub-seasonal, seasonal and decadal timescales). These services are developed in-house via private contracts with companies (e.g. seasonal hurricane prediction platform), funding agencies (e.g. RESILIENCE providing seasonal predictions for wind energy) and collaboration with public administrations. This is the case of the CALIOPE and AIRE CDMX air quality forecast systems, or the two WMO regional centers of sand and dust storms hosted by BSC-ES together with AEMET (the WMO Sand and Dust Storm WAS or the Barcelona Dust Forecast Center-BDFC). ESS also provides knowledge transfer to spin-off companies interested in exploiting operational opportunities. An interdisciplinary team including researchers, science communicators and user-engagement specialists collaborates closely with all the research groups within the department and the support teams at the BSC (technology transfer office, communication and design teams and data visualisation team) to ensure that users remain at the centre of the research process and the outcomes are both useful to and usable by them.

The selected candidate will work with climate predictions and climate projections to co-develop indicators relevant for the needs of the aforementioned sectors. His/her activity will be positioned within the context of WMO's Global Framework for Climate Services (GFCS), whose aim is to advance climate predictions to provide actionable sub-seasonal to decadal climate information to key sectors of society. This position therefore presents the opportunity to work alongside a wide range of leading international climate scientists delivering cutting-edge climate science and climate services across Europe.

The proposed research will be managed through fortnightly meetings with the supervisor to ensure full coherence between the research planned and the general objectives of the department. Regular meetings will take place involving the rest of the department members, especially those in the Climate Prediction and Earth System Services groups, to ensure an adequate integration of this research into the rest of the research carried out in the department. In this context, the applicant will be encouraged to participate in discussions and meetings involving the H2020-funded projects MED-GOLD, VISCA and S2S4E.

Earth Sciences Department

Group Leader: ALBERT SORET

https://www.bsc.es/discover-bsc/organisation/scientific-structure/earth-system-services

Research project/ Research Group description

Project 21:

The ESS group (www.bsc.es/ess) is seeking a specialist in applied economics to develop and implement a robust research to foster the intersection of economics, environmental science and climate services. ESS aims at developing tailored services on weather and atmospheric composition model simulations (focussing on short-term time scales) and climate predictions (focusing on the sub-seasonal, seasonal and decadal timescales). These services are developed in-house via private contracts with companies (e.g. seasonal hurricane prediction platform), funding agencies (e.g. RESILIENCE providing seasonal predictions for wind energy) and collaboration with public administrations. This is the case of the CALIOPE and AIRE CDMX air quality forecast systems, or the two WMO regional centers of sand and dust storms hosted by BSC-ES together with AEMET (the WMO Sand and Dust Storm WAS or the Barcelona Dust Forecast Center-BDFC). ESS also provides knowledge transfer to spin-off companies interested in exploiting operational opportunities. An interdisciplinary team including researchers, science communicators and user-engagement specialists collaborates closely with all the research groups within the department and the support teams at the BSC (technology transfer office, communication and design teams and data visualisation team) to ensure that users remain at the centre of the research process and the outcomes are both useful to and usable by them.

Successful candidates will have a dual passion for financial markets and sustainability as well as demonstrated expertise in quantitative research techniques, including knowledge of leading-edge approaches, sectorial data, climate information, statistical software and academic literature. The candidate will collaborate with the ESS team (postdocs in climate sciences and air quality, social scientist and communication specialists) and relevant stakeholders (energy companies, agricultural enterprises, public administrations, etc.) to bridge the gap between science and its end users in key sectors of society (energy, agriculture and urban development). Special interest in user-engagement processes and knowledge and technology transfer will be valued. Experience in conducting interviews, workshops, and other user-engagement activities to understand the value and the impact of climate and air quality services will be valued.

The proposed research will be managed through fortnightly meetings with the supervisor to ensure full coherence between the research planned and the general objectives of the department. Regular meetings will take place involving the rest of the department members, especially those in the Earth System Services group, to ensure an adequate integration of this research into the rest of the research carried out in the department. In this context, the

applicant will be encouraged to participate in discussions and meetings involving the H2020-funded projects S2S4E and MED-GOLD.

Earth Sciences Department

Group Leader: ALBERT SORET

https://www.bsc.es/discover-bsc/organisation/scientific-structure/earth-system-services

Research project/ Research Group description

Project 22:

The ESS group (www.bsc.es/ess) is seeking for a postdoc in air quality/atmospheric composition/meteorology modelling willing to work together with scientists to do applied research and provide user tailored products for different air quality related projects. ESS aims at developing tailored services on weather and atmospheric composition model simulations (focussing on short-term time scales) and climate predictions (focusing on the sub-seasonal, seasonal and decadal timescales). These services are developed in-house via private contracts with companies (e.g. seasonal hurricane prediction platform), funding agencies (e.g. RESILIENCE providing seasonal predictions for wind energy) and collaboration with public administrations. This is the case of the CALIOPE and AIRE CDMX air quality forecast systems, or the two WMO regional centers of sand and dust storms hosted by BSC-ES together with AEMET (the WMO Sand and Dust Storm WAS or the Barcelona Dust Forecast Center-BDFC). ESS also provides knowledge transfer to spin-off companies interested in exploiting operational opportunities. An interdisciplinary team including researchers, science communicators and user-engagement specialists collaborates closely with all the research groups within the department and the support teams at the BSC (technology transfer office, communication and design teams and data visualisation team) to ensure that users remain at the centre of the research process and the outcomes are both useful to and usable by them.

Successful candidate will support the developments to set up those systems and provide added value products for:
urban development (working in urban environments at high spatial resolution). To gain a better understanding and predicting the spatiotemporal variations of atmospheric pollutants along with their effects upon air quality, weather and climate.
and/or solar energy sector and aviation (providing user tailored indicators). The fellow will work on improving our understanding of aerosol-chemistry processes in the atmosphere through numerical experiments with the MONARCH model. New aerosol and chemistry processes will be implemented and tested in the system to improve user tailored products for the solar energy sector and aviation.

The proposed research will be managed through fortnightly meetings with the supervisor to ensure full coherence between the research planned and the general objectives of the department. Regular meetings will take place involving the rest of the department members, especially those in the Earth System Services and Atmospheric Composition groups, to ensure an adequate integration of this research into the rest of the research carried out in the

department. In this context, the applicant will be encouraged to participate in discussions and meetings involving the H2020-funded project SOLWATT and direct contracts with public administration entities to define mobility measures and air quality plans.

Life Sciences Department

Group Leader: ALFONSO VALENCIA

https://www.bsc.es/discover-bsc/organisation/scientific-structure/life-sciences

Research project/ Research Group description

Project 23:

The Computational Biology group led by ICREA Professor Alfonso Valencia, within the Life Sciences Department at the Barcelona Supercomputing Center (BSC) is seeking a highly motivated post-doctoral researcher to develop machine learning solutions to integrate, reconstruct and analyze epigenetic regulatory networks from high-throughput OMIC data (histone modifications, DNA methylation, chromatin structure and others).
The Computational Biology group has taken a prominent role in the analysis and interpretation of epigenomics datasets in the context of the BLUEPRINT project (http://www.blueprint-epigenome.eu/). In this framework, computational methods have been developed for the study of the 3D genome architecture, the modeling of epigenetic network communication, and the identification of cell type-specific chromatin state determinants and dynamics.
The proposed activity will be centered on integration and analysis of epigenetic data in a network-based predictive framework. The selected candidate will work in a highly sophisticated HPC environment, will have access to systems and computational infrastructures, and will establish collaborations with experts in different areas.

References:

- Ecker S, et al. Epigenetic and Transcriptional Variability Shape Phenotypic Plasticity. Bioessays. 2018 Feb;40(2). doi: 10.1002/bies.201700148.
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- Juan D, et al. Epigenomic Co-localization and Co-evolution Reveal a Key Role for 5hmC as a Communication Hub in the Chromatin Network of ESCs. Cell Rep. 2016 Feb 9;14(5):1246-1257. doi: 10.1016/j.celrep.2016.01.008.
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- Fernández JM, et al. The BLUEPRINT Data Analysis Portal. Cell Syst. 2016 Nov 23;3(5):491-495.e5. doi: 10.1016/j.cels.2016.10.021.

Life Sciences Department

Group Leader: MARIA JOSE REMENTERIA

https://www.bsc.es/discover-bsc/organisation/scientific-structure/life-sciences

Research project/ Research Group description

Project 24:

The Social Link Analytics group led by María José Rementeria, within the Life Sciences Department of the Barcelona Supercomputing Center (BSC), is looking for a highly motivated postdoctoral researcher to develop and applying computational solutions to analyse the impact of projects and organisations in the society.

The general objective of this specific project is to build a Foundations Public Open Data set and analyze the activity of the approximately 10000 foundations working in Spain.

The proposed project will focus on the development and use of tools for text mining, data analysis and data visualization. The selected candidate will work in a highly sophisticated HPC environment, will have access to computer systems and infrastructures and will establish collaborations with experts in different application areas.

Life Sciences Department

Group Leader: VICTOR GUALLAR

https://www.bsc.es/discover-bsc/organisation/scientific-structure/electronic-and-atomic-protein-modeling-eapm

Research project/ Research Group description

Project 25:

Monte Carlo FEP development for Drug Design and Allostery-The Electronic and Atomic Protein Modeling (EAPM) lab at the Barcelona Supercomputer Center, leaded by ICREA Prof. Victor Guallar, in collaboration with the Cardiovascular & Metabolic Disease (CVMD) lab in AstraZeneca (Sweden), leaded by Dr Anders Hogner, seeks for a postdoctoral STARS fellow for the development of novel Monte Carlo Free Energy Perturbation (FEP) techniques. Based on our in house PELE Monte Carlo code, highlighted in the latest international CSAR blind competition as an "outstanding breakthrough" and an "impressive accomplishment", we aim to develop a FEP module to be applied in obtaining protein-ligand relative binding free energies. The methodology will be applied in a real drug design setup at AstraZeneca, involving, in addition, the study of allosteric sites.
We seek a highly motivated researcher with large experience in developing (programming) and applying biophysical methods. Experience with FEP techniques and/or allosteric modulators will be valued.
The fellow will spend part time at both institutions (in Barcelona and Molndal), enjoying the opportunities of top research and industrial environments, with a competitive compensation.

Life Sciences Department

Group Leader: DAVID TORRENTS

https://www.bsc.es/discover-bsc/organisation/scientific-structure/computational-genomics

Research project/ Research Group description

Project 26:

Within the working frame of the Computational Genomics group in the Life Sciences Department, fellows will use bioinformatics and computational approaches to contribute to the understanding of the genomic basis of disease. Our group is interested in developing and applying bioinformatics methodology to answer specific questions on which genomic changes cause which disease, and on the molecular and physiological mechanism behind. As part of the largest and latest initiatives around the world, our group is contributing to the identification of genetic variants associated to the risk of developing complex diseases, like asthma, or diabetes. In parallel, we are also devoting great efforts to cancer genomics, developing tools for somatic variant calling to understand how chromosomal structural variations are affecting tumor formation and progression. This research activity is combined with efforts to translate this methodology into Healthcare systems to contribute establishing the basis of the Genomic Medicine.

Life Sciences Department

Group Leader: JOSEP LLUIS GELPI & SALVADOR CAPELLA

https://www.bsc.es/discover-bsc/organisation/scientific-structure/computational-bioinformatics-node-national-institute

Research project/ Research Group description

Project 27:

Bioinformatics software quality: a text-mining approach for extracting meaningful metrics.

Emergence of new technologies and biomedical problems foster the continuous development of bioinformatics software. However, little is known about how existing software evolves over time. Some of them are maintained by communities; others are discontinued in favor of newer versions and/or approaches; others simply disappear from their initial repositories. Software registries and repositories e.g. GitHub, are a good source of information for keeping track of those changes. However, those resources only offer a partial view of the indicators used to measure software quality. Thus, using text-mining techniques to extract information from software webpages and publications would complement that partial view.

The fellow will work in the constructions of systems to automatically assess the evolution of bioinformatics software in terms of accessibility and usage.

Life Sciences Department

Group Leader: MIGUEL VAZQUEZ

https://www.bsc.es/discover-bsc/organisation/scientific-structure/life-sciences

Research project/ Research Group description

Project 28:

The Genome Informatics unit of the Life Sciences Department is developing methods and infrastructure to assist OMICs analyses for healthcare and basic research projects. The work in the context of precision medicine includes the development of efficient and accurate analysis pipelines that make optimal use of the BSC computational resources with new methodological combining bioinformatics, statistics and machine learning approaches.

The unit is in close contact with groups that have expertise in the relevant application areas from computing to genome projects in the nearby hospitals -with a focus in cancer. Therefore, the work will consist in a combination of programming, project development, application design, basics of statistics and machine learning, data analysis and visualization.

Life Sciences Department

Group Leader: MARTIN KRALLINGER

https://www.bsc.es/discover-bsc/organisation/scientific-structure/life-sciences

Research project/ Research Group description

Project 29:

Our main focus is to improve access, integration, processing and understanding of biomedical and clinical unstructured data of relevance to patient safety, clinical research and precision medicine. This implies developing, applying and evaluating computational resources that empower systematic extraction of information contained in textual data. The main target data types of interest to our group include basic biomedical research literature, clinical texts generated by healthcare professional and user-generated content produced by patients such as social media.

By applying biomedical and clinical text mining systems, we are able to expose associations between heterogeneous classes of biomedical entities. These include genes, sequence variants, chemical/pharmacological substances, diseases, symptoms and adverse events.

Our research activity uses machine learning, cognitive computing and natural language processing approaches together with terminological resources and ontologies as a basis for multilingual document processing, with a particular focus on Spanish, Catalan, Galician, Basque and English texts.

The main objective of this position will be the construction of Interoperable and integrated text processing components and advanced applications of text and data mining for clinical research.