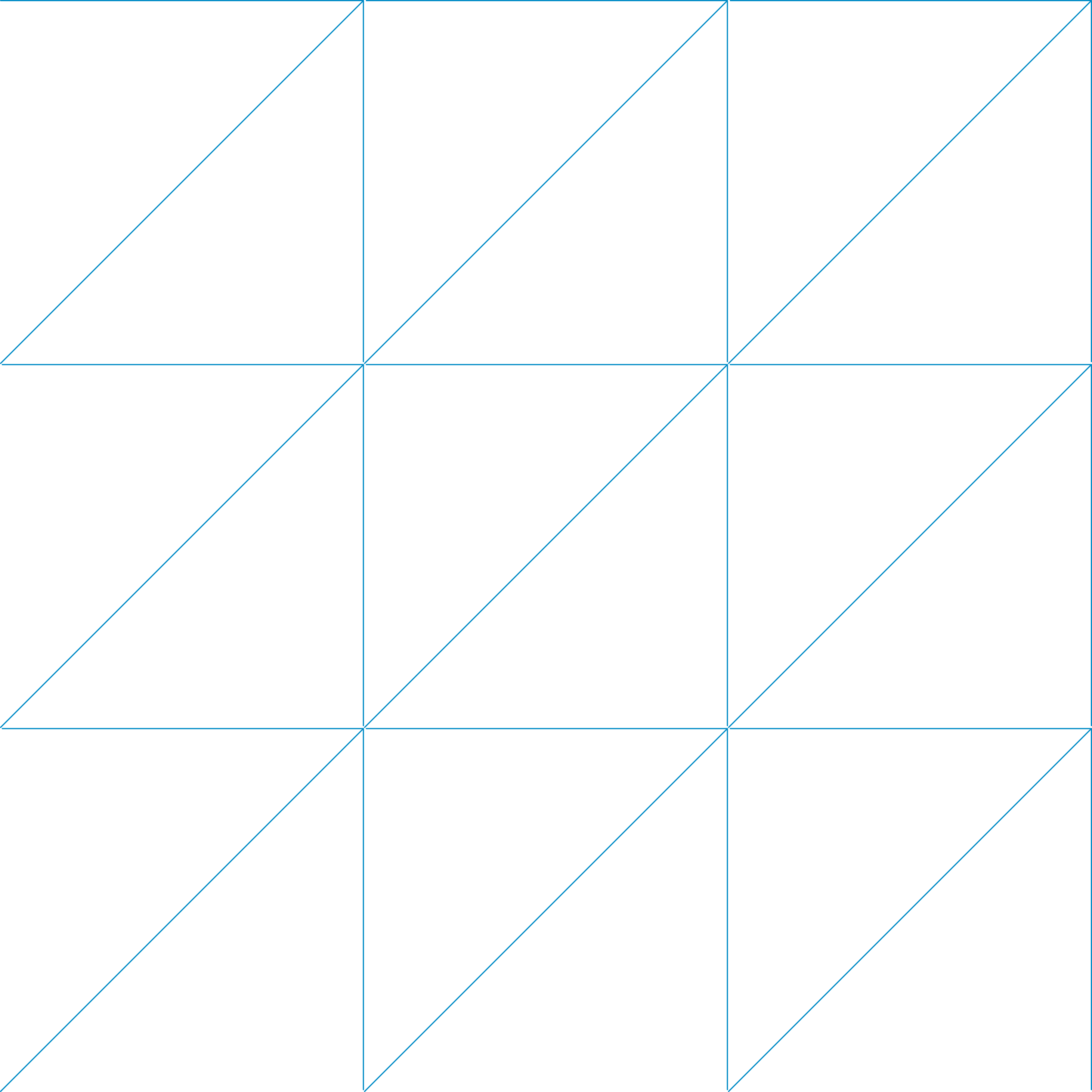
basque center for applied mathematics

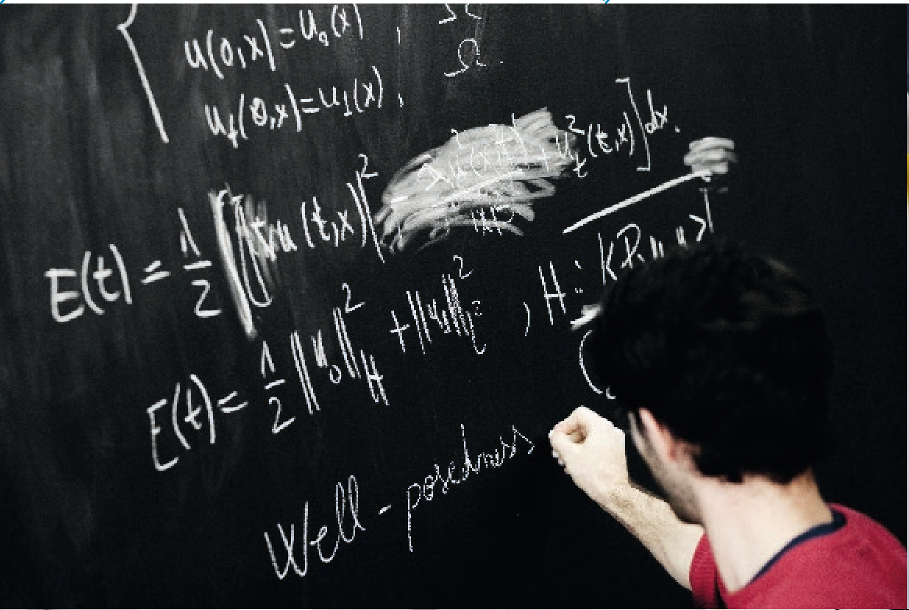
MATHEMATICS THE LANGUAGE OF SCIENCE



basque center for applied mathematics

EXCELENCIA
SEVERO
OCHOA


bcam
bcam




bcam


Equilibrium condition

PRESENTATION

"If people do not believe that mathematics is simple, it is only because they do not realize how complicated life is." Von Neumann, 1947

The only universal language

BCAM is a world-class interdisciplinary Research Center in the field of Applied Mathematics that was founded in 2008 as a Basque Excellence Research Center (BERC), with a focus on interdisciplinary research in mathematics, as well as training, attracting talented scientists, and promoting scientific and technological advances worldwide.

BCAM scientific activities are organized into Research Lines working in relevant areas through highly competitive projects developed by BCAM researchers. With the mission *"mathematics in the service of society"*, we are committed to establishing links and collaborations with industry, R&D companies and social institutions, in order to transfer our excellence research in Applied Mathematics to diverse areas (industrial, energy, materials, health, social, ecological, financial...), contributing in a sustainable manner to XXI century societal challenges.

BCAM got in 2013 the Severo Ochoa Excellence Research Center distinction as one of the best centers in the world in its field. The road ahead presents many challenges, such as consolidating and expanding our research teams, developing new programmes and activities and strengthening links with international and local partners.

ADOLFO MORAIS EZQUERRO
Basque Government Education
Linguistic Policy and
Culture Vice-Counsellor

LUIS VEGA GONZÁLEZ
Scientific Director

Basque Smart Specialization Strategy (PCTI 2020) couples research and innovation, with its emphasis on excellent science, industrial leadership, tackling societal challenges. The goal is to ensure that the Basque Country reaches sustainable economic growth, produces world-class science, removes barriers to innovation and makes it easier for the public and private sectors to work together in delivering innovation. BCAM, as a world class center for applied Mathematics, is aligned with this strategy. BCAM's high contribution to excellence pillar research and its potential for knowledge transfer have been widely recognized, being a key stakeholder for the internationalization of our R&D activities.

The effort made by BCAM researchers since its establishment has already produced some significant results. The Severo Ochoa distinction is a great achievement and a great step forward that will allow us to strengthen our position as an obliged reference of Applied Mathematics in Spain, and consolidate BCAM as one of the most relevant institutions of the field in Europe. To achieve this objective, we will be faithful to our compromise to carry out research at the frontier of mathematics, always within the bounds of excellence. We also aim to maintain our commitment towards mathematics in the service of society, to ensure that the effort made when providing BCAM with public funding is a resounding success.


$M \in \mathbb{N}$ with $M > 0$
$(\Phi, \Psi) \in Y_M$
$\Omega_M = \{\Theta_0, \Theta_1, \dots, \Theta_M\}$
$P_M, Q_M : [-\tau, 0] \to$
$0 = \Theta_0 > \Theta_1 > \dots > \Theta_{M-1} > \Theta_M = -\tau$
$Y_M := \mathbb{R}^{\Omega_M / \{0\}} \simeq \mathbb{R}^M$
$Z_M := \mathbb{R}^{\Omega_M} \simeq \mathbb{R}^{M+1}$
$\Phi := (\Phi_1, \dots, \Phi_M) \in Y_M$
$\Psi = (\Psi_0, \Psi_1, \dots, \Psi_M) \in Z_M$
$\mathcal{A}_M \simeq \mathcal{A}$
$\Rightarrow$ The eigenvalues
$\lambda \in \sigma(\mathcal{A})$
$\lambda_M \in \sigma(\mathcal{A}_M)$

SCIENTIFIC TOPICS INDEX

We develop new computational technologies in order to increase the reliability of computer simulations.

01.1

SIWP

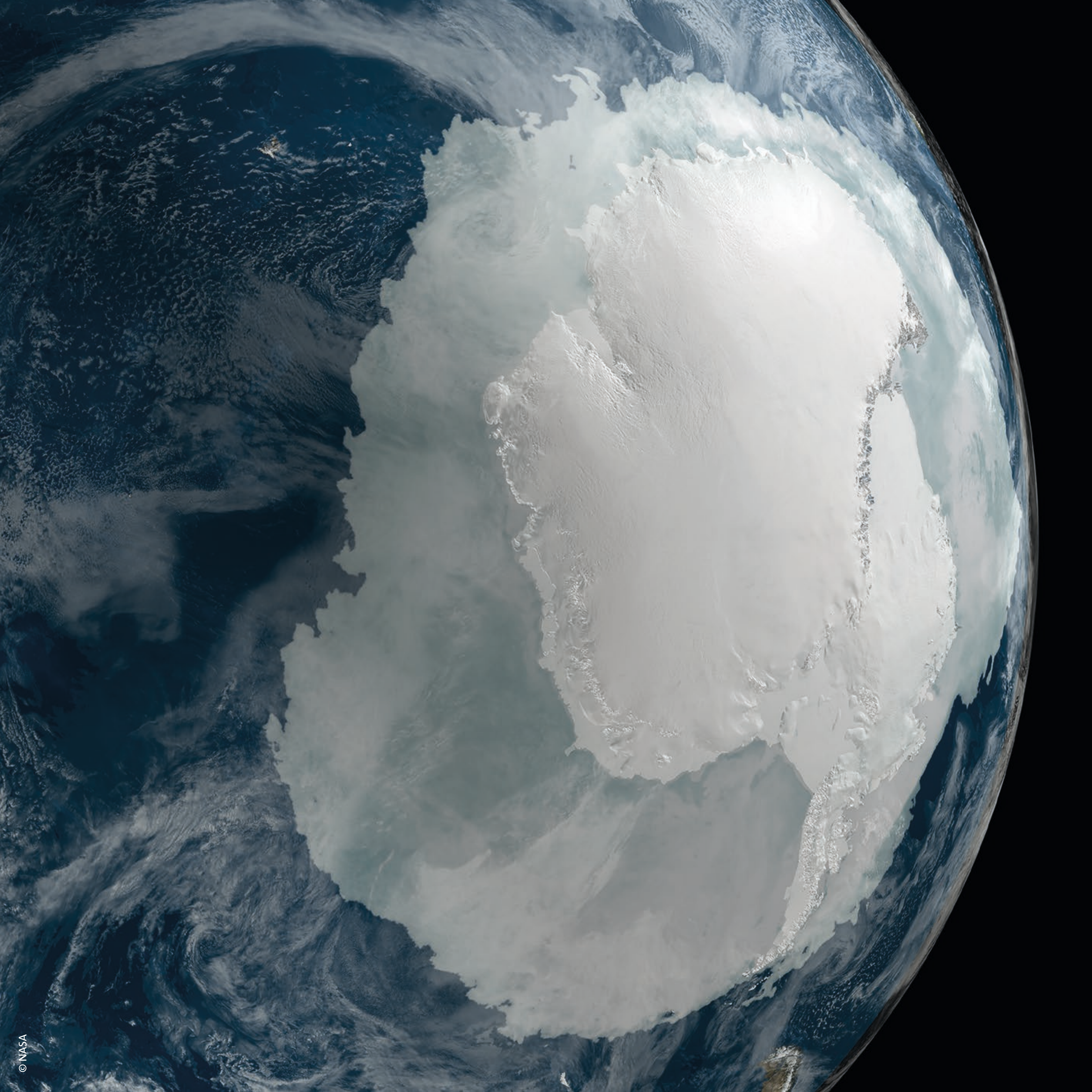
Simulation of Wave Propagation

Leader: David Pardo
Ikerbasque | UPV-EHU | BCAM

01

CM

Computational Mathematics



By combining classical algorithms and recent trends in modern numerical analysis, we construct robust and efficient methods to reliably simulate a wide range of applications.

01.1

SIWP

Simulation of Wave Propagation

OBJECTIVE

We design, analyze, implement and optimize numerical schemes for mathematical models arising from real-life applications. We also develop new advanced finite element based simulation methods to efficiently solve challenging industrial applications.

DESCRIPTION

In order to obtain reliable algorithms, and therefore valid and trustworthy simulations, a strong mathematical framework is of paramount importance. In this context, we devote part of our work to the mathematical analysis of modern numerical methods (advanced finite element methods and discontinuous Petrov-Galerkin methods among others) to be applied to both stationary and time dependent problems.

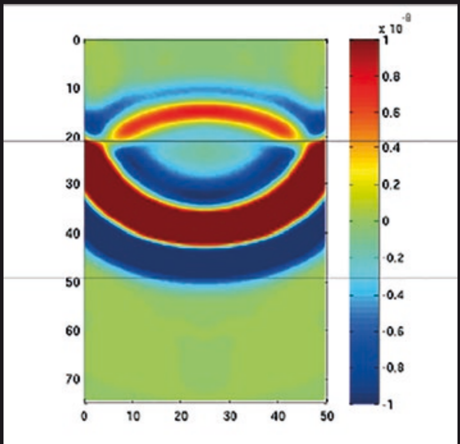
Although aspects such as mesh generation and convergence are classical in the area of computational mathematics, they are still very important, as they provide an a priori knowledge about the behaviour of the proposed algorithms. We are also interested in adopting some recent trends in numerical analysis, such as reliable a posteriori error estimates and efficient mesh adaptivity procedures to reduce the computational costs of the simulations. By combining these two theoretical aspects when designing the new algorithms to be implemented, we expect to obtain robust and efficient numerical methods to simulate a wide range of applications.

APPLICATIONS

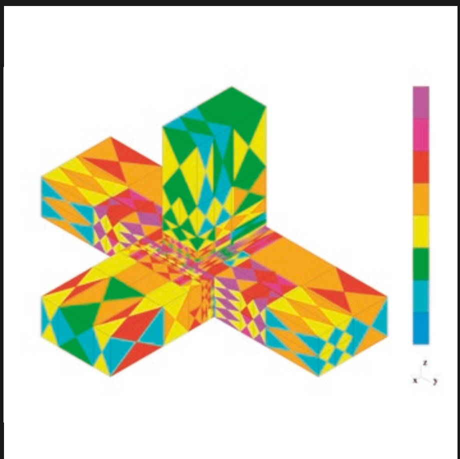
We work on characterizing the materials that compose the Earth´s subsurface, which is essential to, among others: (a) predict earthquakes, (b) find and extract precious minerals such as gold, copper, and hydrocarbons (oil and gas), (c) determine the geological history of our planet, and more recently (d) store CO2 underground to minimize the effect of pollution. The most common way to determine such materials is by sending electromagnetic and acoustic waves underground, measuring the signal recorded in a nearby receiver, and employing sophisticated numerical methods to properly interpret those measurements, revealing the subsurface materials through which that wave has been travelling. Therefore, it is crucial to dispose of robust and efficient solvers for the wave equation, in time or frequency domain. At BCAM, we design new algorithms, and build simulation software that allows us to model the electromagnetic and acoustic waves that are sent underground, and we also develop new

SIMULATIONS

Propagation of acoustic wave in 2D stratified medium.



Final grid obtained with an advanced Finite Element Method.



methods for interpretation of the recorded measurements, providing a high-resolution characterization of the materials composing the Earth´s subsurface. Among the main methods developed at BCAM for that purpose, we encounter advanced grid-generation methods, multi-goal oriented adaptive methods, high-order finite element methods, stable discontinuous Galerkin and discontinuous Petrov-Galerkin methods, parallel multi-physics algorithms, etc.
Another application of interest is the deformation of polymers and ductile metals, when subjected to extreme tensile extension. In order to observe and analyze these deformations, we combine numerical techniques - such as mesh generation and refinement, interpolation polynomials, Newton-like methods - with non-linear elasticity concepts to compute approximate minimizers for the energy of the materials.

We are also concerned with the numerical solution of magnetohydrodynamic problems. Their study is motivated, among others, by technological applications like driving a liquid metal through a magnetic field in order to produce electricity and by their role in the description of space (within the solar system) and in astrophysical plasmas (beyond the solar system). We use mesh-free methods to design numerical schemes that overcome the instability observed in problems with high Hartman number, a typical situation for real-life applications.

Other potential applications of our work are modelling of fuel cells and computational anatomy. Fuel cells, devices which convert chemically bounded energy (e.g. hydrogen) directly into electricity, are related to one of the main problems faced by civilization, that is, the increasing energy hunger combined with limited resources and decreasing reserves.

Regarding computational anatomy, one of its main purposes is the measurement and statistical study of anatomical variations in organs, notably in the brain and the heart to detect the appearance of tumors, plasticity, and the absorption of anatomical structures.

Industry 4.0: Pushing current limits in fluid modeling, simulation and optimization.

01.2

CFD

Computational Fluid Dynamics

Leaders:

Johan Jansson BCAM | KTH

01

CM

Computational Mathematics

We develop innovative CFD methods and platforms providing accurate, reliable and efficient solutions for complex industrial problems.

01.2

CFD

Computational Fluid Dynamics

OBJECTIVE

We aim to develop new mathematical methods and robust numerical massively parallel software to solve complex and large-scale challenging problems that rise from many sectors including aerospace, automotive, ventilation, power generation, chemical manufacturing, polymer processing, petroleum exploration, medical research, meteorology and so on. The methods are implemented in Computational Fluid Dynamics (CFD) platforms BBIPED (high order finite volume) and FEniCS (adaptive stabilized finite element methods) to meet the demanding industrial requirements in terms of accuracy, efficiency, cost-effectiveness, and user-friendly graphical interface. We also aim to promote the CFD discipline in the Basque country through courses, seminars and workshops and trainings for students and industrial staff.

DESCRIPTION

CFD is the discipline of mathematics that aims to model and simulate fluid motion and its interaction with the environment. CFD has made significant inroads in industrial applications thanks to the advent of affordable high-performance computing (HPC) along with powerful visualization tools that have widely opened the door to large-scale applications. However and despite this significant progress, modelling some complex phenomena that occur at very small scales like turbulence and aeroacoustics is still a big challenge.

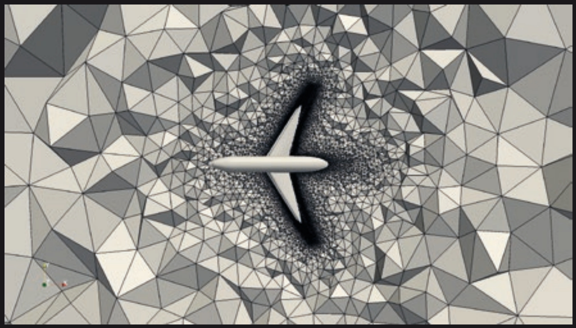
To tackle these challenging problems two highly efficient CFD platforms are developed and are in continuous progress:

— **BBIPED:** in this platform the state-of-the-art approaches are implemented with many innovative methods like the virtual multiple rotating frame technique that reduces drastically the processing time of turbo-machines simulation. And others are in progress like turbulence modelling using techniques from homogenization theory that will allow simulating turbulence with high accuracy and reasonable time processing since the model will not require any additional closer equations and no calibration parameters to tune.

— **FEniCS:** in this platform we use a parameter-free adaptive finite element methods (AFEM) based on quantitative a posteriori error estimation that is considered leading in the field of turbulence simulation. We develop adaptive stabilized finite element methods based on a posteriori error estimates and a Unified Continuum model for fluid-structure interaction with moving meshes/basis functions as a general framework for interface tracking. To achieve

SIMULATIONS

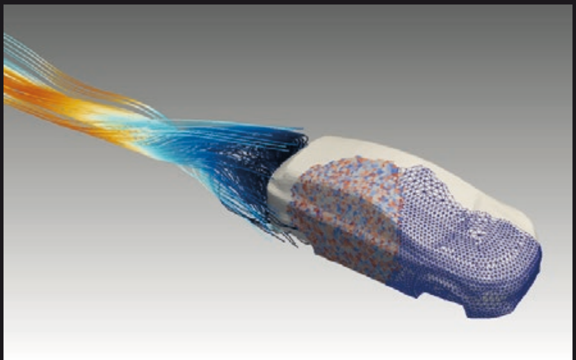
Aircraft: slice aligned with the angle of attack showing the tetrahedra of the starting mesh (A) and finest adaptive mesh (B) for α=18,5°.



A

B

Stream lines of turbulent flow over a car simulated with BBIPED.



software generality and efficiency we use code generation and develop high-level parallel frameworks with good scaling on supercomputers. We have received a PRACE Tier-0 supercomputing grant for our FEniCS-HPC framework, which is the highest level in the EU, and our project is the only PRACE project in the field of mathematics.

↗ APPLICATIONS

Fluids are everywhere around us, from the tap water in our houses to the blood in our vessels. CFD is a core element in many domains which are of a vital importance to humanity, such as biomedicine, meteorology, oceanography, aeronautics, naval architecture, acoustics and turbomachinery. Beyond its impact on industry, CFD has an important role to play in the advancement of science. CFD also impacts directly our daily life through for instance the aerodynamic optimization of vehicles that results in fuel consumption reduction and increasing passengers comfort. We can also mention noise reduction for turbo-machines in airports, factories and tunnels.

In this context and by means of BBIPED tailored developments to turbomachines, we achieved a highly accurate industrial BALTOGAR turbofans simulation using an innovative approach based on virtual multiple rotating frame and an automatic fan parametrization. We also aim to apply our developments to the laser beam deposition process, a gas-particle model along with an original immersed domain optimization technique.

By using FEniCS we have been able to produce breakthrough results in the simulation of a full aircraft as part of a benchmarking workshop organized by NASA and Boeing. Using our novel parameter-free adaptive finite element methodology for turbulent flow has given excellent agreement with experimental data. Another main application is the simulation of turbulent fluid-structure interaction with contact in the vocal folds in the EUNISON FP7 FET-Open project which aims to computationally model human voice generation from fundamental mechanics.

We have also achieved interesting results when applying our methodology to the turbulent mixing in the jet of a gas burner, which has allowed us to start a collaboration project with Bosch and Siemens Home appliances group (BSH) in Santander, Spain.

Many open challenges in life sciences modeling require efficient algorithms and robust supporting theories.

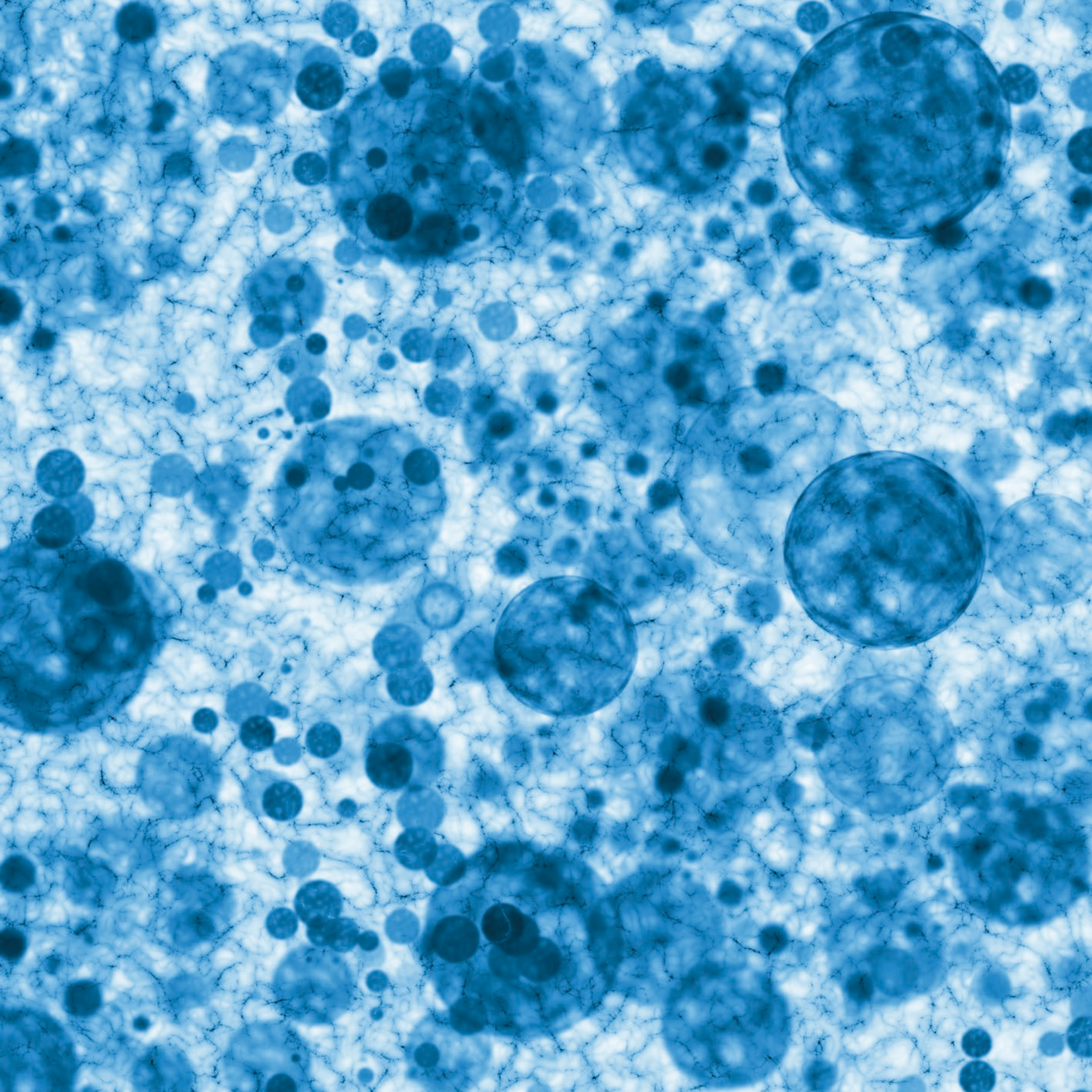
02
M3A
Mathematical Modelling with Multidisciplinary Applications

02.1
MSLMS
Modelling and Simulation in Life and Materials Sciences

Leader: Elena Akhmatskaya
Ikerbasque | BCAM

02.2
MMB
Mathematical Modelling in Biosciences

Leader: Luca Gerardo-Giorda
BCAM



Our goal is efficient and detailed simulation of complex phenomena stemming from real life problems in biology, medicine, public health and society.

02

M3A

Mathematical Modelling with Multidisciplinary Applications

OBJECTIVE

Our objectives are effective modeling and detailed simulation at different scales of extremely large and complex systems and phenomena stemming from real life problems in biology, medicine, public health and society. We are interested in both applications and methodology, to devise reliable predictive tools for biomedical applications, material science, and conservation biology. Focus is also on application of high performance computers (HPC) to problems currently beyond the capacity of existing methods.

DESCRIPTION

Quantitative predictive simulation of complex biological and physical processes, required for solving some of the pressing issues facing society today, is still beyond reach despite recent progress in hardware development. The challenge lies in developing novel algorithmic approaches and improved computational models, in order to fully exploit the capabilities of modern HPC.

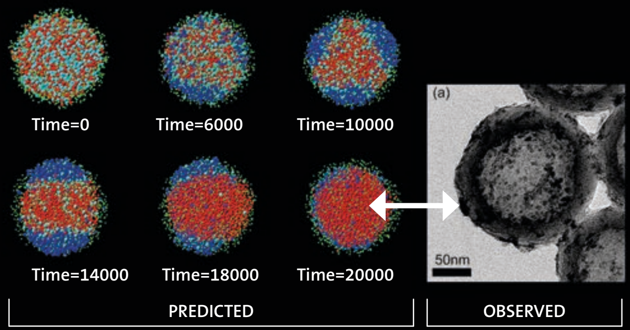
M3A researchers are working on inventing novel numerical algorithms and sampling techniques making possible the accurate modeling of complex systems of various natures, which are currently beyond the capabilities of the existing modeling approaches.

Powerful algorithms are implemented in user-friendly state-of-the-art computer codes and made available to a broad user community, involving applied mathematicians, researchers, medical doctors and workers of hi-tech industries. Exploitation of the software helps to solve some outstanding problems arising in Biosciences, Materials Sciences, Geophysics or Economics. Ultimately, the results will be translated into contributions to public health, medicine, engineering, industry, environment and society.

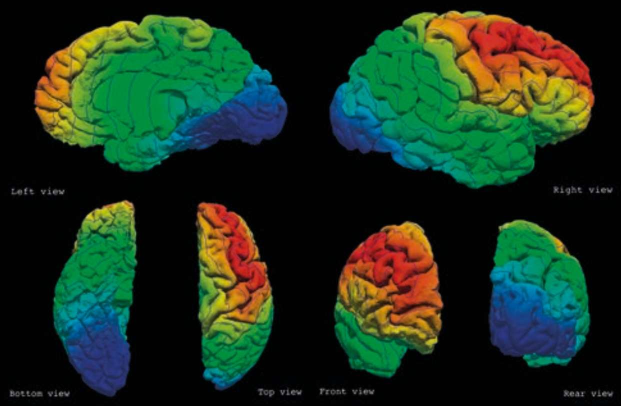
Development of novel sampling methods combining stochastic Markov Chain Monte Carlo with deterministic Hamiltonian Dynamics is one of our long standing research interests. The methods (some of them are patented) aim to overcome the deficiencies of conventional sampling techniques. We work on extension of the methods to a range of simulation scales and statistical ensembles as well as on further improvement of their efficiency through adopting novel adaptive schemes, numerical integrators and parallel algorithms. The developed methodologies are implemented in the in-house unique efficient multiscale multipurpose sampler – a highly parallelized simulation package allowing for optional simulation of complex systems and rare events at atomistic, meso- or multiscales using the state of the art sampling technology.

SIMULATIONS

Dynamic modeling of the morphology of latex particles



Finite element simulation of the Cortical Spreading Depression



Another important area of our research is patient-specific simulations of the cardiovascular system, obtained by coupling numerical simulation with individual anatomies reconstructed from imaging, and integrating such models with available measurements. Such strategy, called in silico and progressively used in the clinical practice, aims to provide complementary tools for understanding pathologies, designing new devices and optimizing therapies.
Computational models have been a supporting decision tool for cardiovascular surgeons in the last decades. The possibility of performing virtual surgery on a patient-specific geometry is fundamental to have additional, noninvasive, insights at both diagnostic and prognostic level.
In addition, we develop the computational kits, which couple the novel numerical methodologies with the in-house software and are tailored to particular applications. This includes among others efficient solvers for electrocardiology and a high-resolution heart model, based on clinical data; Bayesian characterization of brain fMRI; modeling and numerical simulation of the spreading depression in the cerebral cortex; numerical algorithms for analysis of chemical reactions; coupling atomistic and mesoscale hybrid Monte Carlo simulations in drug design; development of the multiscale stochastic reaction diffusion model for prediction of polymer morphology development; combining ensemble based Bayesian approaches with Hamiltonian Monte Carlo in reservoir simulations.

↗ APPLICATIONS

The primary applications of the methods, models and software developed in M3A are patient-specific simulation of cardiovascular and brain activities; virtual screening for drug design; self-assembly in biological and chemical processes; modelling electroactive energy materials; uncertainty quantification in reservoir simulation and simulation of synthetic markets.
We work in close collaboration with medical doctors (BioCruces, Hôpital de Bordeaux), biophysicists (Oxford), mathematicians (Valladolid, UPV, Potsdam, INRIA, Emory, Santa Barbara), material scientists and chemical engineers (POLYMAT, CIC-EnergiGune), chemists and physicists (UPV, St Andrews), computer scientists (BSC), and statisticians (Sussex, Rhode Island).

Towards mathematical understanding of theories of Physics.

03.1
QM
Quantum Mechanics

Leader: Jean-Bernard Bru
Ikerbasque | UPV-EHU | BCAM

03.2
SP
Statistical Physics

Leader: Gianni Pagnini
Ikerbasque | BCAM

03.3
STAG
Singularity Theory and Algebraic Geometry

Leader: Javier Fdez. de Bobadilla
Ikerbasque | BCAM

03
MP
Mathematical Physics

We ease interdisciplinary connections breaking the language barrier among fields.

03
MP
Mathematical Physics

↗ OBJECTIVE

At the interface between mathematics and physics is the so-called Mathematical Physics which includes, Quantum Mechanics and Statistical Physics, recently we have incorporated Algebraic Geometry and Singularities, a more theoretical research line with applications in this area.

Our aim in **Quantum Mechanics** is to understand from a mathematical perspective how the same microscopic laws yield a large number of macroscopic behaviours. Particular attention will be paid to the macroscopic properties of interacting quantum systems.

In the field of **Statistical Physics**, our main goal is the development of statistical approaches to model natural phenomena with both theoretical and social interest. In particular, the research is focused on processes characterized by the random propagation of fronts.

In **Singularity Theory and Algebraic Geometry** we study the geometry of Singularities arisinf in Algebraic Geometry and Differential Topology and qualitative changes that occur in the dependence of phenomena on parameters, when the parameters meet singular points.

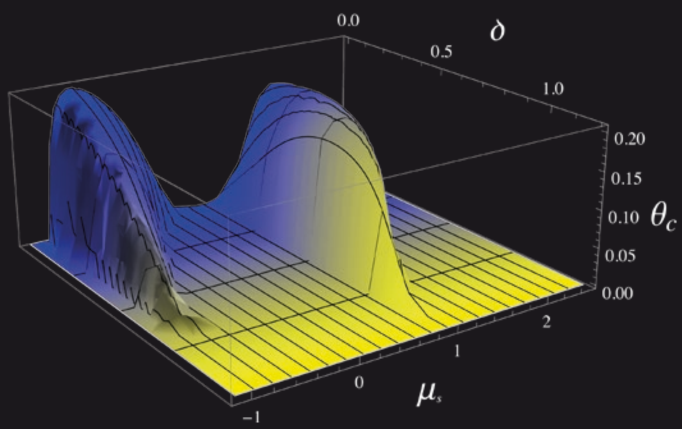
↗ DESCRIPTION

The question of the microscopic origin of macroscopic laws like in (classical) electricity theory is a borderline problem which belongs to rigorous Quantum Statistical Mechanics. Many effective theories of Physics are indeed not understood from first principles of Quantum Mechanics. For instance, Ohm's law (electricity theory) is maybe the most known law and it is surprising that significant progresses on its mathematical derivation from Quantum Mechanics have been made only in the last years, while Ohm's law has been experimentally verified in a quantum world only in 2012.

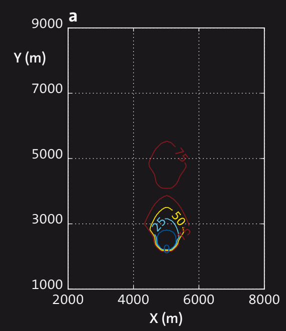
Natural phenomena with a complex behaviour that require a statistical analysis can be investigated by using methods developed in Statistical Physics. One of the most widely used techniques for tracking front propagation is the so-called Level-Set Method (LSM). However, many applications require to track fronts embedded into a random environment. The LSM is generalized to describe such random situations according to the probability density function of the displacement of interface around the average frontline determined by the ordinary LSM. The correct determination of the probability density function, is therefore of paramount importance for any applications.

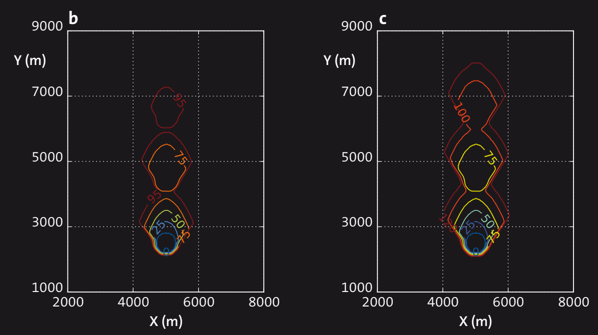
SIMULATIONS

Illustration of the superconducting phase as function of temperature, chemical potentials and energy gap of a microscopic two-band model based on the structure of energetic levels of holes in CuO2 conducting layers of cuprates.



Simulation of wild-land fire propagation including turbulence and fire-spotting effects





Singularities arise naturally in a huge number of different areas of mathematics and science. As a consequence Singularity Theory lies at the crossroads of the paths connecting applications of mathematics with its most abstract parts. For example, it connects the investigation of optical caustics with simple Lie algebras and regular polyhedra theory, while also relating hyperbolic PDE wavefronts to knot theory and the theory of the shape of solids to commutative algebra. Algebraic geometry classically studies solutions of systems of polynomial equations in several variables multivariate polynomials. It is even more important to understand the intrinsic and geometric properties of the totality of solutions of a system of equations, than to find a specific solution.

↗ APPLICATIONS

The past decade has seen a drastic increase in interest in quantum phenomena, driven by experiments on superconductors, Bose-Einstein condensates (2001 Nobel Prize in Physics) and electronic properties. These quantum systems are already paving the way to a brand new technological branch (atoms lasers, atom chips, etc). Our studies focus on the most popular theories to describe such quantum properties. This makes them to be of high interest both for the challenging future applications of quantum technologies and for the analysis of quantum phase transitions like in high-Tc superconductivity.

Methods of Statistical Physics can be applied for the development of approaches to model random front propagation in real world situations of environmental and social interest. In particular for turbulent premixed combustion, which is the characteristic technology of future combustion devices since it permits a strong reduction of NOx emission with respect to the conventional combustion technologies, and for wild-land fire propagation.

Algebraic Geometry and Singularities have applications in robotics, analysis of gravitational lenses, computer vision, coding theory and criptography. Even the most abstract parts of algebraic geometry find applications in string theory, a branch of theoretical physics which seeks for a unification of gravity with the other 3 fundamental forces.

Describing efficiently real life phenomena using PDE models.

04

APDE

Analysis of Partial Differential Equations

04.1

WAVE

Linear and non-linear Waves

Leader: Luis Vega
UPV-EHU | BCAM

04.2

HA

Harmonic Analysis

Leader: Carlos Pérez
Ikerbasque | UPV-EHU
BCAM

03.3

APAN

Applied Analysis

Leader: Arghir Zarnescu
Ikerbasque | BCAM

We explore and exploit the deep connection between PDEs, Harmonic Analysis, and Applied Mathematics.

OBJECTIVE

We quantify the interaction of waves that propagate in a dispersive media, either linear or non-linear, where singularities are present. Our approach is a mixture of techniques of Fourier Analysis and Partial Differential Equations.

We study some of the central operators and some of the main analytical tools from Harmonic Analysis to understand properties of the solutions of Elliptic Partial Differential Equations.

We study major current PDE models that have physical and biological relevance. We analyse their consistency and determine their broad predictive capabilities and limitations.

DESCRIPTION

Waves are ubiquitous in Nature as they can describe the most diverse phenomena. At the same time they suppose a challenge from the mathematical point of view due to the richness and complexity of their interaction either in linear or non-linear media. Thanks to the ERC advance grant HADE we will analyse, using techniques of Harmonic (e.g. Fourier) Analysis, different phenomena concerning waves as: the Kelvin waves that travel along vortex filaments and whose interaction is quite likely behind the chaotic behaviour of turbulent fluids; the relativistic quantum waves as those describe by Dirac Hamiltonians; and the uncertainty principle of quantum mechanics one of the deeper consequences of the wave description of the quantum world.

We consider Calderón-Zygmund Operators and their commutators with BMO functions making special emphasis on their interaction with the Ap theory of weights. Fundamental results and methods of this theory like extrapolation or factorization are used. We also consider Potential Operators and Poincaré type inequalities, core objects in the theory. We study properties of generalized (degenerate) Poincaré type inequalities where intrinsic aspects of the underlying geometry play a main role. These inequalities are intimately related to the key Poincaré-Sobolev inequalities via the “self-improving” property of these objects. Tools such as the Good-lambda technique or some of the decomposition formulae from modern Harmonic Analysis are essential methods to be explored. We will also consider multilinear aspects of the theory.

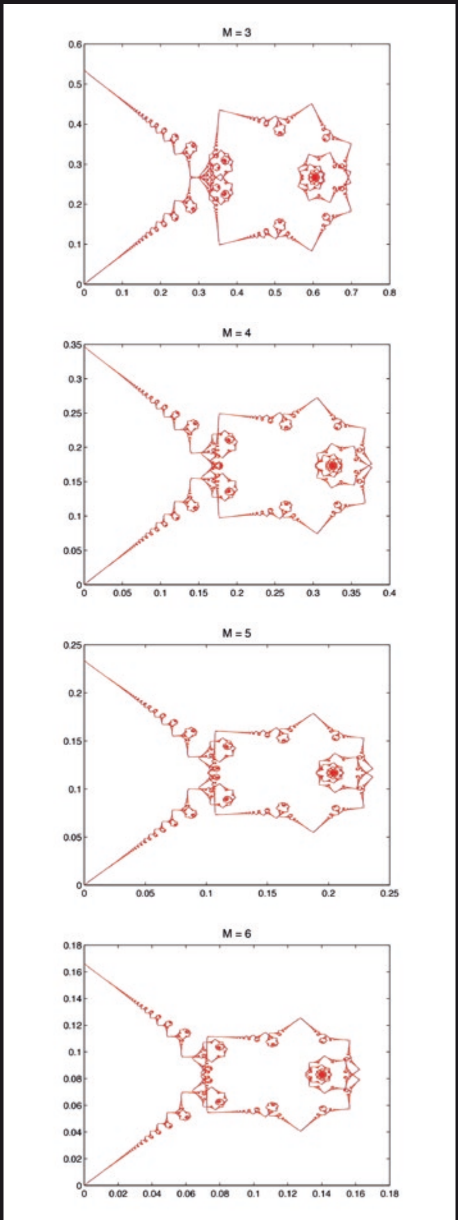
04

APDE

Analysis of Partial Differential Equations

SIMULATIONS

Trajectory according to Vortex Evolution Equation of one vertex of regular polygons with different number of sides.



The attempt to describe efficiently real-life phenomena leads to mathematical models, often expressed in terms of PDEs, capturing the essential features of the phenomena. Usually these models have their own mathematical limitations and are valid only in certain ranges of parameters while outside these ranges predict unphysical behaviours. The overall aim is to determine the major mathematical features of the models.

↗ APPLICATIONS

The understanding of the fundamental principles that control relevant phenomena in physics as the interaction of waves will rise applications in real life. The description of turbulence, that is considered by many the most important unsolved questions of classical physics, is a remarkable example of such a situation. In some of our recent results about the Vortex Filament Equation we have discovered that, due to the intrinsic stochastic nature of turbulence, we can give efficient algorithms to generate pseudo-random numbers. This could eventually become of use in different scenarios such as numerical simulations (e.g. for the Monte Carlo method), electronic games, and cryptography.

One of the goals is to prove regularity estimates for degenerate second order differential operators in divergence form having a positive matrix with degenerate least and greatest eigenvalue and to study properties of subelliptic operators or fractional powers of the sublaplacian on Heisenberg group. We plan also to derive Hardy-type inequalities with maximal functions as a bonus for non-standard operators as well as estimating the negative eigenvalues of Schrodinger operators.

The most interesting and poorly understood PDE models are those that involve nonlinear aspects. Each nonlinear PDE model often exhibits its own specific features and the overall focus of current research is on the study of those models of most relevance and applicability. Among these are: the equations describing fluids (Navier-Stokes equation), quantum effects (Schroedinger equations), complex media (such as liquid crystals) and sophisticated novel materials (like shape-memory alloys or nematic elastomers).

A huge amount of knowledge is hidden in the data, waiting for being extracted and exploited.

05
DS
Data Science

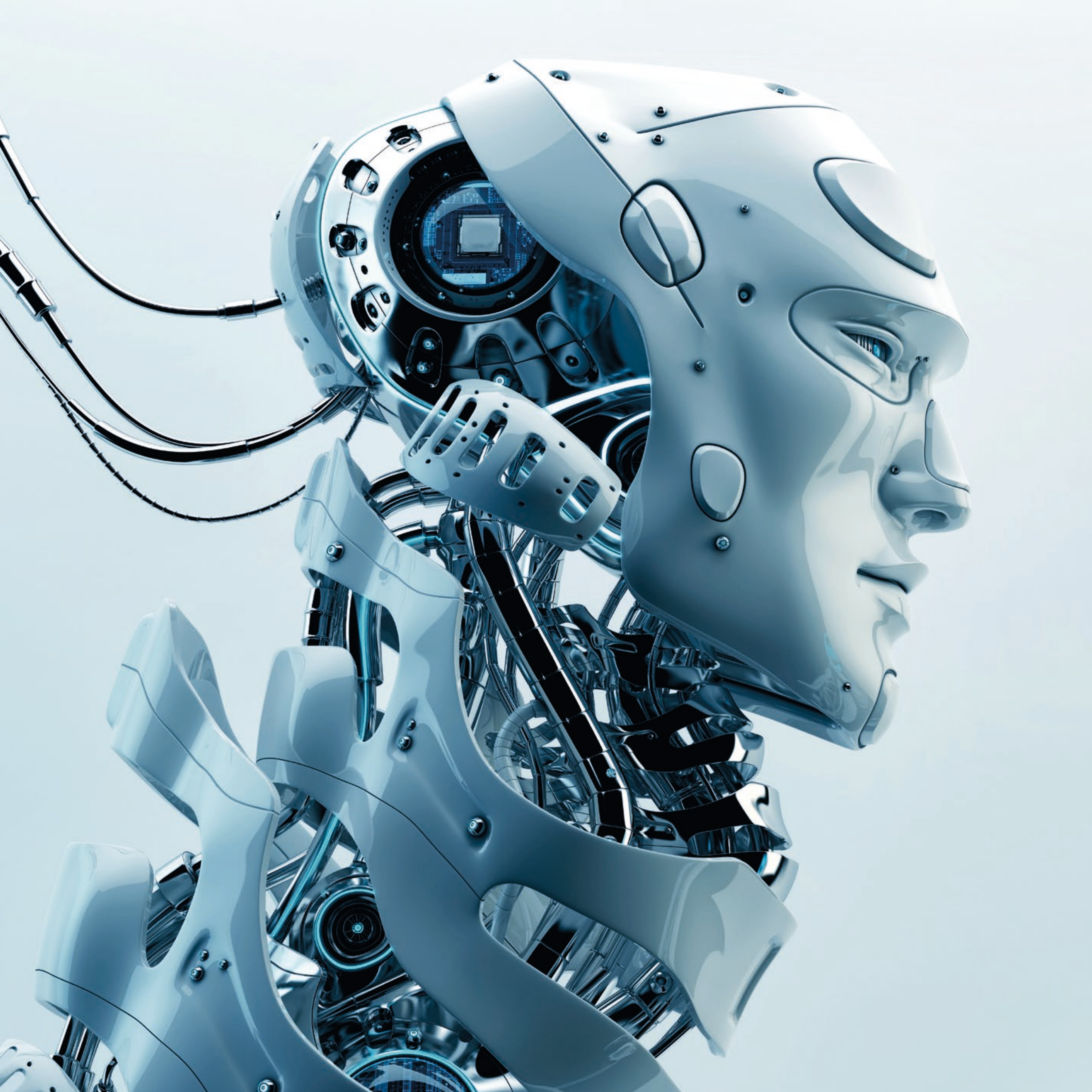
05.1
HEUR
Heuristic Optimization

05.2
AS
Applied Statistics

Leader: Dae Jin Lee
BCAM

05.3
ML
Machine Learning

Leader: Jose Antonio Lozano
UPV-EHU | BCAM



The increase in data generation (Big Data) has made indispensable the development of new statistical and machine learning methods and algorithms for knowledge extraction and optimization.

OBJECTIVE

Nowadays, we are surrounded of devices able to capture enormous amount of data. Many branches of science and businesses have passed from a data-scarce situation to a tsunami of information. The knowledge extraction from these vast collections of data has received increasing importance. On the other hand, optimization problems in areas such as logistics, scheduling or planning have enormously increase in size that make them impossible to solve to optimality.

Our first main goal is to create innovative statistical and machine learning models, inference methods, computational algorithms and visualization tools for the analysis of massive data. These models can be used to solve domain-specific problems that can be grouped into supervised classification, clustering, regression, ranking, etc. Our second aim is to develop new metaheuristic optimization algorithms able to reach good solutions in bounded computational time.

Computational and Statistical methods are required for accessing, managing, integrating, analysing and modelling datasets of diverse nature and complexity. In this sense the scientific contributions in the data analysis are twofold theoretical and practical. The theoretical contributions consist of developing novel mathematical theories and models able to extract knowledge from data, together with the design and analysis of general purpose or domain specific efficient and scalable algorithms for learning statistical models. From the optimization point of view, our aim is to study computational and theoretical aspects of combinatorial optimization and to develop new heuristic optimization techniques able to find good solutions in reasonable computation time.

The practical contributions are the application of the developed techniques to different fields such us, biology, medicine, bioinformatics, ecology, transportation, etc.

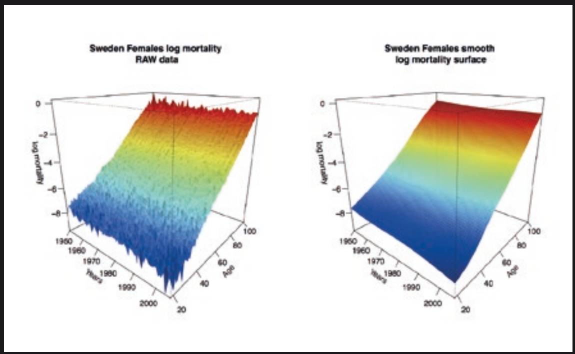
DESCRIPTION

The rapid growth in the size and dimensionality of data sets is driving the need for novel statistical models and methods that can handle these new data structures. This new framework is concerned, not only with the volume of data, but also with the complexity, variety of the type of information available, correlation structures, and efficient and computational algorithms to solve complex problems throughout mathematical models.

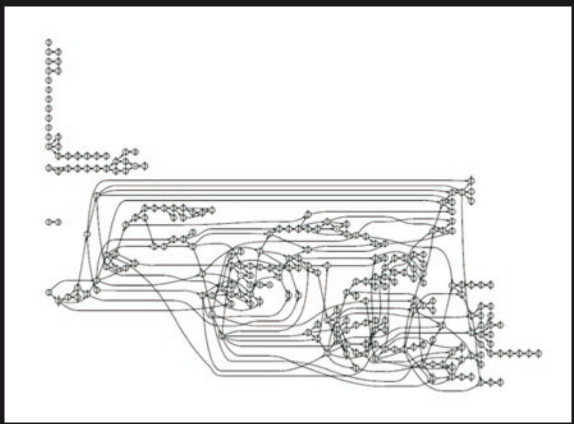
In the applied statistics field, the main topic of our research are semi-parametric regression, multidimensional smoothing, (Bayesian) hierarchical models, mixed and random effects models, design of

SIMULATIONS

Raw and smooth death rates in logarithmic scale using Penalized splines for Poisson counts. Sweden females, ages 50-100, 1950 to 2006.



Structure of a Bayesian network learned from arrhythmia data set by means of a hill-climbing algorithm guided by the BIC score.



experiments and ANOVA, spatial and spatio-temporal modelling, functional data analysis, computational statistics, and data visualization methods and tools.

Regarding Machine learning, we work on probabilistic graphical models (PGM), mainly focused on the automatic learning of PGMs from data. PGMs can be used for extracting knowledge from data, for reasoning under uncertainty and for simulating domains without an explicit physical model. PGMs can be used to perform efficient probabilistic reasoning and, as decision support systems. In addition, they are suitable to deal with many statistical problems such as supervised classification, clustering and ranking.

Finally, in the optimization area, we plan to develop new metaheuristic algorithms based on Evolutionary Computation and particularly Estimation of Distribution Algorithms. In addition we will explore hybrid algorithms that combine heuristic methods with exact methods: branch & bound and branch & cut methods. Finally research will be done in the Bayesian approaches to optimization.

APPLICATIONS

Our research provides concepts and methods that will be applicable in many fields which demand a wide variety of data modelling and computational tools for the analysis of complex problems. The classic application areas have been robotics, medical and biological domains, epidemiology, environmental sciences, genetics, business, demography, engineering and finance. Due to the increase in the rate of acquisition of data in the last few years, big data or massive data problems arise in fields from particle physics and astrophysics to e-commerce, social media and marketing.

Biostatistics concerns with the application of statistical methods to medical, biological and health related problems (e.g. medical statistics, clinical trials, or epidemiology).

Regarding machine learning, two of the most known applications of statistical models are Supervised Classification (naturally applied as a decision support tool in medical domains - diagnosis and prognosis) and Clustering (commonly applied in marketing segmentation).

The main applications related with the optimization techniques include logistics (vehicle routing, orienteering problem), planning (crew scheduling, timetabling), scheduling (aircraft landing, flow shop), packing (container loading), etc.

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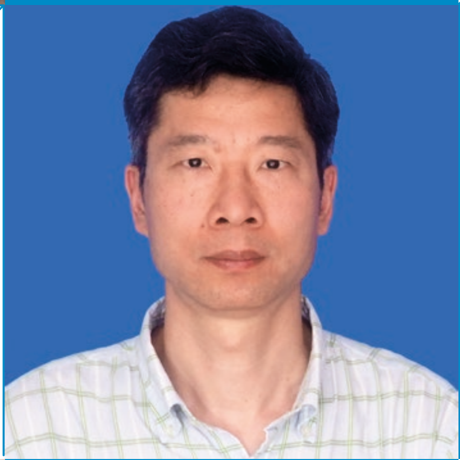

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