

WHITE PAPER AP21

APPLIED MATHEMATICS

Credits: Paragraphs 1.STATE OF THE ART and 4.EMERGING RESEARCH CHALLENGES have been built on the basis of the results of the online consultation on Mathematics carried out in 2016 by the DG CONNECT (European Commission Directorate General for Communications Networks, Content and Technology) in the context of a more general consultation aimed to prepare the Horizon 2020 Work Programme 2018-2020. As reported in “Mathematics for Europe”, June 2016 (copyright: European Union).

EXECUTIVE SUMMARY

Mathematics is a fundamental science with extreme versatility, which is nowadays used in a range of frameworks that extends well beyond the traditional ones, such as physics and engineering. Its use encompasses biomedical science, environment, social sciences, industrial processes, administration, complex systems and many other fields. To be understood, modelled and managed, a world which is more and more digitalized requires an increasing formalization. The ever expanding use of mathematics stems from the combination of powerful computational systems and humongous quantity of data, while the challenges which mathematics faces today are leading to an expansion of its disciplinary foundations, which, in turn, results in an ever increasing reliability and methodological adequacy.

The research activities carried out in the institutes which are contributing to the AP Applied Mathematics, besides the natural interaction with the ICT sector, require a mathematics that, unlike the traditional academic discipline, can cover the whole pipeline of applied research, from the real life problem to its formalized modeling, followed by the development of ad hoc solution methodologies, the realization of a computational framework, with the engineering of the algorithms and, finally, the processing and interpretation of the results. The researchers at CNR bring forward a mathematics that is a driving force, able, with the outcome of their research, to anticipate and steer the needs of the different applications.

The goal that we are pursuing is twofold. On the one hand, we aim at developing, analysing and implementing innovative methodologies in different fields of applied mathematics. On the other hand we want to study its application in different frameworks: in those fields where the problems are already posed in “mathematical form”, with the development of alternative, more robust and efficient formulations, the use of state-of-the-art methodologies and the “certification” of the results; and in fields where the problems are not yet described in “mathematical form”, with a multidisciplinary approach and the contribution of our expertise in modelling and, afterwards, the development of analytical and computational solution tools.

1. STATE OF THE ART

Mathematics is a prerequisite for contemporary development in most fields of science. It is essential for both the exploitation of big data and the development of HPC towards exascale and quantum. At the same time, these developments are also enablers for new mathematics.

Data analysis, Topological applications, Mathematics for HPC, Complexity, Finance mathematics, and MSO (Modelling, simulation and optimisation) are important areas in being. Biomathematics is also emerging as a new prominent area.

At present time, most results are concentrated on new and emerging mathematical areas needed for the development of HPC, data or better simulation tools. Among these, we find tropical mathematics (algebra and geometry), algebraic-topological-geometrical methods for data analysis, approximate inference methods, stochastic geometric mechanics, integral biomathics, theory of evolving systems, etc.

Also probability, statistics and financial mathematics are indispensable, with new challenges requiring new approaches. Block-chain, trading algorithms, actuarial challenges of tackling big data and its implications for needs for inverse probability theory approaches, are certainly important for the society at large.

Artificial intelligence, robotics and complexity theory as a whole are also fields that require very high level mathematical input and are very important for Europe and for the European Science and Innovation.

The latest publication by the European Science Foundation on “Mathematics, its use and benefits for Europe” highlights success stories on the collaboration of mathematics with industry. Remarkable improvements have been possible in the design, planning and implementation phases of the industrial or service processes, leading to considerable savings and an increase in productivity.

Various areas are listed:

- automotive industry (software for simulation of spray painting, improved automotive injectors, designing oil filters, accelerated simulation, acoustic car design, computation of optical free-form surfaces);
- manufacturing (numerical simulation for the aluminum industry, imbalance estimation in rotating machinery, modelling and optimal control of chemical mechanical planarization, anti-reflection coatings, modelling plasma PVD, improvements in semiconductor crystal production, numerical simulation of metallurgical processes in silicon production, optimal utilization of colored gemstones, simulation of polymeric textile products, modelling and analysis of rotary fiber spinning);
- aerospace and electronics (modelling and simulation of spacecraft charging, flow control of an air duct, aero-engine nacelle acoustic treatments, reduction of testing by developing new ways of simulation, low cost airborne laser fly, simulation of stochastic radar signals, optimization of satellite coverage, simulating rowing boats, waves for ship-simulation, better prediction and understanding of rogue waves, sails modelling, mathematical modelling of complex materials in underwater sonar systems, optimization algorithms in electronics design automation, mathematical modelling of charge transport in semiconductors, online simulation of 3D nano-optical components);
- energy (bentonite buffer in nuclear waste management, intelligent video understanding applied to plasma facing component monitoring, modelling coal combustion, optimal flames in industrial furnaces, optimizing a complex hydroelectric cascade in an electricity market, mathematical models for oil pipelining, improving the simulation of multiphase flows in pipelines, intelligent agent based modelling and simulation of electrical grids, a kinetic model of blast furnace automation, numerical modelling of heterogeneous porous media, aero-acoustic virtual design of exhaust systems);
- environment (modelling and simulation of environmental problems, predicting climate change, solving underground water problems, simulation and optimization of waste water filtration, solar reflector design, simulation of a moving bed reactor used in the pulp and paper industry, dynamic image based lighting for highly realistic lighting in building design);
- health (optimization of radiation therapy, simulating atrial fibrillation, realistic modelling of human head tissues exposure to electromagnetic waves, mathematical modelling of a decontamination process, mathematical modelling of an ultrasound sensor for bioprocesses, minimal paths and virtual endoscopy, simulation of a bone-prosthesis system, unravelling the genetic code, forecasting for urgent medical care call centers, 3D X-ray imaging for dentists, computer simulations in electro-cardiology, non-Fickian diffusion in polymers and medical applications, statistical testing of molecular motion inside living cells, non-invasive test for monitoring diabetes, early cancer detection by proteomics fingerprinting);
- services (tool for population pharmacology, shopper behavior modelling, generation of assignments of products to consumers, geo-temporal exploitation and analysis platform, analysis and forecasting the evolution of human potential and the job market, the use of queuing theory to increase the effectiveness of physician staffing in the emergency department, air elimination in milk pump systems, optimal portfolio mix using insurance market data, new approaches to reinsurance risk calculation, use of mathematics for transport networking, improving cable network capacity, making smart phones even smarter);
- transport and logistics (optimal trip planning in the presence of random delay, aircraft icing solutions, optimization of the emergency management systems, optimization of public transport systems, forecasting model selection in fast moving consumer goods supply chains, increased efficiency in air traffic control, truck load analysis, calibration procedure for a height measurement system for excavators, crew rostering (scheduling), preventive maintenance optimization of trains air conditioning systems, optimization in sea logistics, control of navigable rivers, liner network modelling, contributing to the building of the digital

society);

- other domains (optimal financial portfolios, financial derivatives pricing, pricing model of catastrophe bonds with complete calibration procedure, quantifying the liquidity premium in bond spreads for insurance liability valuation, modelling and forecasting stock price behaviour in high frequency trading, the resource valuation and optimization model, realistic assessment of financial products, model based optimum design of experiments, solution and model appraisal in reservoir inverse problems using global optimization methods, modelling and assessment of maintenance efficiency of repairable systems, optimization of electricity production, virtual piano based on mathematical modelling, secure communication for automatic teller machines, uncertainty assessment in high-dimensional nonlinear inverse problems, modelling and detection of realistic human actions in video, real-time video distortion correction, cognitive vision, handwriting recognition).

Interestingly, the largest computations in fluid mechanics in the world and one of the biggest computational capacities nowadays is in Hollywood (US). The film industry is running enormous simulations of flows, for instance to represent realistic-looking sea, waves, rivers, or to imitate real-life behaviour and produce other remarkable visual effects.

2. CONTRIBUTION TO THE RELEVANT SCIENTIFIC AREA

Max 10000 characters (the limit includes spaces)

Describe the main AP_CNR activities and its positioning in the relevant area wrt the previous chapter

Modellistica e calcolo scientifico

IAC

Mathematical and numerical modelling

in the context of *Continuum Mechanics and Fracture, Biology, Medical Sciences, Physical Chemistry, Ecology* ..., either as fundamental research and for problem solving.

Mathematical modelling, numerical methods, optimization techniques and simulation for particle systems and fluids in classical, quantum and relativistic conditions with applications in: *Theoretical, Applied and Computational Fluid Dynamics, Statistical Mechanics, Porous Media, Multi-Phase Flows, Material Science, Engineering, Cosmology, Environment (Hydrology, Glaciology, Pollutant extraction from soil, Collective behaviour of intelligent individuals, Traffic flow, E-Mobility) at any scale, from Macro to Atomic Scale, Nuclear and Sub-Nuclear.*

Qualitative study and numerical analysis

of Mathematical Models (linear and nonlinear partial differential, integral, integro-differential and discrete systems).

Numerical methods, algorithms and High-Performance Software

for Sparse Linear Algebra, Predictive Simulation Science.

Data, signal and image analysis

Variational methods, multi-resolution analysis, non-linear approximation for *image analysis*.

Mathematical models, accurate and efficient algorithms and software for *data analysis* and *signal processing*.

IASI

Biomathematics

Simulation and analysis of stochastic differential equations models of integer and fractional order; \mathbb{R}^n Structured Partial Differential Equations models; Statistical Estimation of parameters for deterministic models and SDE models

IMATI

Analysis of PDEs

Optimal Transport problems and their entropic regularizations; analysis of transport equations with low regularity coefficients; non-local conservation laws, i.e. involving averaged velocity fields, which appear in models of both pedestrian and vehicular traffic; boundary conditions for systems of conservation laws; *Novel multifunctional materials* such as shape-memory and magnetostrictive alloys.

Numerical Methods for PDEs

Treatment of complex geometries (the virtual element methods. Isogeometric analysis). Mesh adaptivity based on geometric and PDE-based criteria (e.g., geometric mesh quality, approximation accuracy, numerical stability)

Geometric and numerical methods for the multi-resolution representation and approximation of geometric data and scalar/vectorial design of preconditioners (domain decomposition, multigrid).

Uncertainty Quantification: collocation methods for UQ; Sparse Grids/Multi-Index Stochastic Collocation.

Computational topology and geometry

Geometrical and topological methods cellular and simplicial complexes, discrete exterior calculus, differential topology, Morse theory simplicial homology groups computational algebra (splines, B-splines, extended Hough transforms) to curve fitting over (non-planar) surfaces.

Image processing

Development and comparison of image metrics, Wavelet methods, Image registration, Image classification, Image similarity assessment.

ICAR

Mathematical modelling and Scientific Computing

Focus on *Problem Solving* with methodologies that include computational simulation, scientific modeling, analysis, processing, and management of complex, heterogeneous, and large data sets. These methods integrate high performance computing (HPC) and distributed computing, with Computer Science, Applied Mathematics, and Statistics expertise. By appropriately integrating the methodologies with the knowledge of different application domains, we provide a new and more effective perspective for the analysis of real-life problems and the interpretation of results.

IIT

Algorithms and computational mathematics

This research group investigates models and algorithms for the solution of complex problems arising in some topical applicative areas, such as *Web Information Retrieval*, *Computational Biology*, algorithmic for *Wireless Networks* and *Smart Mobility*. These activities are also complemented with basic research activities in the field of numerical linear algebra.

ISTI

Computational mechanics

ISTI carries out research and software development in the field of *mechanics of solids*, with a particular focus on structural engineering, with the development of the Finite Element code NOSA-ITACA.

Computational topology and geometry

Analysis of visual data based on concepts from differential geometry, differential topology and algebraic topology; Group-invariant Persistent Homology and its use for Topological Data Analysis.

Sparse Image Representation and Dictionary Learning

Efficient representation of high dimensional data generated by a multivariate linear model, driven by a small number of basis or regressors.

INM

Computational fluid Dynamics

Advanced numerical techniques for *Marine Hydrodynamics applications*. Lagrangian and hybrid Lagrangian-Eulerian particle methods; Diffused Vortex Hydrodynamics; flows characterized by breaking waves and high free-surface deformations; flows around complex bodies

New models for the *Optimization of Ship hull* novel design-dimensional space reduction methods for shape optimization in ship hydrodynamics and multi-physics problems. Dynamic/adaptive meta-modeling and machine learning techniques and global derivative-free bio-inspired optimization algorithms have been

Evolution of viscous Newtonian fluids over a *superhydrophobic surface*

Hybrid BEM/RANS coupling Development of the CFD solver Xnavis/PRO-INS for the *Hydrodynamic Analysis of Marine Propellers*.

Development of high-Reynolds model for LES Analysis of the performances considering high Reynolds flows around naval geometries (submarines). Development of wall model functions for high-fidelity LES simulations.

Development of a non-standard 'immersed boundaries technique' in the curvilinear viscous high Reynolds number solver Xnavis.

Development of a general purpose gas-dynamic solver including high order spatial and temporal discretization schemes, AMR techniques, immersed boundaries approach and two phase flow capabilities.

Optimization and Discrete Mathematics

IAC

Mathematical optimization, control, game theory and decision-making science.

Discrete mathematical modelling, discrete structures, applications of graph theory, meta-modelling, study of computational complexity of algorithms, approach to constrained and unconstrained problems, methods of linear and nonlinear mathematical programming, methods of linear and multilinear algebra and numerical linear and multilinear algebra.

IASI

Optimization

A Two-Stage Robust Optimization scheme to shift scheduling and nurse-to-patient assignment and studying different versions of robust network loading problems.

Network Optimization problems: analysis of theoretical properties and development of solutions algorithms for network loading, capacitated network design, hierarchical networks, wireless problems.

Bilevel optimization problems in job shop and network design.

Mixed-Integer Nonlinear Optimization with Semicontinuous Variables: Perspective Reformulations, solutions methods, semi-infinite reformulations, quadratic reformulations.

Direct Methods: Derivative-Free solution methods for Nonlinear Optimization problems. These are methods that can be applied when derivative are either not available or very time-consuming, e.g. in black-box optimization and simulation-based optimization.

Discrete Mathematics

Polyhedral descriptions of the Stable Set polytope for claw-free graphs and other classes of graphs; *Solution methods for the Max-Cut problem*: different approaches for dense graphs of medium size and for sparse graphs of very-large size graphs.

Graph coloring problems: theoretical properties and solution algorithms for node coloring, edge coloring, total coloring, sum coloring.

Hierarchical Scheduling: a new model and a 2-approximation LP-based algorithm for makespan minimization.

Natural Optimization Algorithms. Rigorous mathematical analysis, that in a network setting, Physarum polycephalum's dynamics are able to compute almost-optimal solutions to shortest paths and network transshipment problems on any weighted network. New Nature-inspired solution methods for Linear Programming and Convex Optimization.

Modellistica stocastica e analisi di dati

IAC

Applied and theoretical probability

Dynamical processes on *Random Graphs*, gaussian and poissonian approximation of *Random Walks* and point processes.

Data and Signals

Statistical models, algorithms and software for *data analysis*.

Accurate and efficient algorithms for *signal processing*. Information Theory, Big-data analysis, multivariate analysis, dimension reduction, Bayesian statistics, machine learning; computational pipelines for analysis and integration of data from Next Generation Sequencing.

IMATI

Space and time stochastic processes

Stochastic differential equations and nonparametric methods. Markov and point processes for industrial and environmental applications. Enhancements to self-exciting and self-correcting models for seismic applications. Stochastic differential equations and dynamic stochastic programming for population dynamics simulation.

ISTI

Stochastic modeling of complex systems

Stochastic models of random (mono- or multi-dimensional) signals generated by *complex self-organizing systems* (e.g., biomedical signals), with particular attention to *intermittent (possibly hidden) behavior*.

System Theory and optimal control

IASI

System Theory and optimal control

State prediction for nonlinear stochastic differential systems; Block-tridiagonal state-space realization of Chemical Master Equations (CME); Modeling biological timing and synchronization mechanisms by means of interconnections of stochastic switches

ICAR

Optimization techniques for *Machine Learning (ML), Multiple Instance Learning (MIL)*

IEIT

Modeling, analysis, Inference and optimization, and *control of dynamics over networks and Markov random processes.*

3. IMPACT

Max 7000 characters (the limit includes spaces)

Describe AP_CNR current impact at scientific, industrial, social and political level. Consider both national and international perspective.

Examples of the impact of the CNR activity in Applied Mathematics is given by the following applications

IAC

- For the *Design and manufacturing of new soft mesoscale materials* with applications in *Tissue engineering, Photonics*, an ERC senior grant (COPMAT) has been awarded to S. Succi. This is supporting a research group working on the full-scale mathematical modelling and numerical simulation at nanometric resolution of microreactors for the design and synthesis of new tunable porous materials.
- Mathematical simulation tool with patient-specific calibration in support to eco-doppler investigation for *Early non-invasive diagnosis* of anomalies in fetal circulation.
- Mathematical and numerical modelling of the coupled system, Atmo-, Hydro-, and Cryosphere, for prognostic and diagnostic study of *Climate Change impacts*.
- In Epidemiology, accurate forecast of an *Epidemic behavior* and more appropriate *Control actions* are the main target. A contribution in this direction to the development and analysis of mathematical models for waterborne infections and diseases is expected, possibly with the inclusion of random effects.
- Mathematical models and algorithms for the description and control of flows describing *Collective behaviour of intelligent individuals (cells, cars, people)* in heterogeneous environments.
- Mathematical modelling and support to signal and data processing for *Complex Biological Systems* (for disease diagnosis, medical therapy upgrade, process understanding at intra/extra-cellular and systemic level) .
- Mathematical models and computational methods for data analysis, signal processing and image analysis applied to *Cultural Heritage, Environment (remote-sensing data for Earth Observation and atmosphere modelling, applied meteorology, climatology, data from atmospheric multiple scattering, pollutant detection), Security and Defence, Health and Biology, Material Science, 3D Printing*
- Partial differential modelling and numerical simulation for chemical damage forecast of artifacts aimed at conservation and protection of *Cultural Heritage* .
- Processing, exploration, analysis and knowledge extraction from *Complex, Etherogeneous and Multi-Dimensional Data*.
- Mathematical models and methods for *Economics, Actuarial Sciences and Finance*
- Application of optimization methods in support of decision-making in the context of *Social Systems, Intelligent Transport, Advanced Sustainable Logistics, Management of Safety, Security and Emergency, Supply Chain in Agri-Food*
- Mathematical models for *Social, Biological and Technological Networks*, and quantitative study of the main performance measures.

IASI

Applications of technologies developed at IASI include:

Optimization Applications in *Power Energy Production, Network Design Problem, Sensor/Facility Localization, Portfolio Optimization*, and others.

Modeling the probabilistic behavior in *biochemical networks*.

Modeling of *biological timing and synchronization mechanisms* by means of interconnections of stochastic switches.

IMATI

Application areas of the methodologies developed at IMATI include:

- *Life sciences*: simulation of blood flow in the brain, simulation of tissue perfusion in the eye, simulation of the electric activity of the heart, study of gene regulatory networks
- *Automotive industry*: study of contact problems for tyre design
- *Smart materials*: simulation of shape memory and magnetostrictive alloys, simulation of electronic nano devices
- *Project and process management*, in different frameworks, from ecology to Smart-care and Smart-living applications.
- *Seismology*: Analysis of earthquakes catalogs for hazard assessment
- *Environment*: Design of energy efficient buildings, groundwater flows, basin compaction
- *Additive manufacturing*.

ICAR

- *Processing and analysis of biomedical images*: bioinformatics and computational biology (analysis and integration of data from high throughput sequencing experiments, microscopy, and spectrometry); high throughput screening of stem cells in microscopy images; segmentation of melanomas in dermoscopic images; moving object detection for video surveillance and for characterizing the vitality of treated cells in electron microscopy videos.
- *Optimization for Machine Learning*: optimization techniques, such as Support vector machine and bundle methods for nonsmooth minimization problems, play a relevant role in Machine Learning (ML), since most ML problems are formulated as mathematical programming problems, and need the employment of efficient and specialized optimization algorithms. Multiple Instance Learning (MIL): the objective is to categorize bags of points (instances). Differently from supervised classification problems, where the label of each point in the training set is known, in a MIL problem only the labels of the bags are known, whereas the labels of the instances are unknown. Different mathematical programming models have been proposed such as mixed integer nonlinear programming models and a nonconvex nonsmooth unconstrained optimization ones.
- *Non-smooth optimization*: Wireless Sensor Coverage problem, non-smooth optimization for wireless sensor networks.
- *Transportation and logistics*: Optimization models for planning of urban transit accounting for guide automation, high quality user preferences, and multimodal integration; Optimization models for the management of multimodal container terminals account for zero-inventory logistics.

IIT

Models and algorithms for the solution of complex problems arising in some topical applicative areas, such as *Web Information Retrieval*, *Computational Biology* (Biological sequences and networks analysis/classification; Diseases classification and gene expression profiling), algorithmic for *Wireless Networks* and *Smart Mobility* (Car Sharing, smart intersections, self-driving vehicles).

ISTI

- Applications to *structural health monitoring of historical masonry buildings* and their dynamic identification.
- *Computer Vision and Computer Graphics* applications: 3D shape analysis in digital anthropometry, for the development of health monitoring systems, 3D Digital Fabrication, environmental sensor monitoring. The applications include the virtual restoration and inpainting of degraded manuscript images. Applications were carried out in *brain research* (sleep, consciousness).

INM

- *Marine hydrodynamics applications*: energy dissipation of marine flows characterized by breaking waves and high free-surface deformations.

A new hybrid Lagrangian-Eulerian approaches have been devised: in these schemes the standard mesh-based solvers have been coupled to particle methods in order to retain the advantages of both approaches and tackle complex problems of involving vorticity generation and free-surface deformation.

Another class of particle methods, the Diffused Vortex Hydrodynamics, has been developed and validated for simulating flows around complex bodies at intermediate Reynolds numbers, with specific focus on the wake generated past bodies.

4. EMERGING RESEARCH CHALLENGES

Max 1000 characters (the limit includes spaces)

Describe how AP_CNR is planning to address the emerging challenges of the relevant scientific area, how cooperates on solving the open issues and how contributes to the design of the future

- Modelling and simulation of:

natural phenomena, competitive species and biological invasions, engineering processes across large ranges of scales (*combining stochastic and deterministic approach, new computational methods and tools*); life cycle of industrial products and systems for new solutions/services (*combining physics-based modelling with data-based one*).

- *Stochastic geometric mechanics.*

- *Biomathematics* for new implementations and new applications.

- Getting the most from increasing amount of data in health, mechanics and industry, economics, environment (*inverse problems*).

- Decision making under risk/uncertainty in crime prevention, climate change, migration and defence (*efficient algorithms, optimization of big data sets*).

- Image data manipulation (*quantitative analysis*).

- Real-time monitoring of data stream (*data reduction, handling of different sources/forms of data*).

- Complex and CPU-time consuming measurement processes (*validation, verification, uncertainty estimate*).

5. CONCLUSIONS

Max 2500 characters (the limit includes spaces)

Mathematics is recognized today as essential and indispensable for addressing the major challenges in science, technology and society.

The envisaged changes in key technologies for present and future HPC systems will have significant impact on the development of scientific computing applications. New mathematical methods, numerical analysis, algorithms and software engineering for extreme parallelism are being addressed in order to take real advantage from the new systems as it is stressed in the European Technology Platform for HPC (ETP4HPC) Strategic Research Agenda.

Faced with the growing wealth of data on social, technical, environmental, economic, ecological, and technological systems, new and sophisticated mathematical tools are required for these data to help us tackle pressing societal challenges, provide us with the necessary technological advantages and approach new and further frontiers of knowledge.

It is worth noticing that current developments in big data analysis and HPC's mathematical basis have shown that even existing areas of mathematics formerly deemed merely theoretical, such as algebra and topology, are now very important for these fields. Similarly it is impossible to predict now what mathematical areas should be in the focus, as well being exploitable in 50 years.

Mathematicians will be essential for identifying the potential of emerging and existing mathematical fields, amongst other areas, for the development of exascale and quantum computing, analytical and simulation tools to meet the future environmental, societal and industrial challenges.

Quite importantly, the need for collaboration and increasing convergence between different mathematical disciplines as well as between mathematics and other sciences is definitely evident.

PROJECT AREA 21: APPLIED MATHEMATICS

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