DISMA Excellence Project 2018-2022

The main scientific themes

June 15, 2018

Preamble

The Department currently has a well-recognized role on the national mathematical scene, and also enjoys a good position on the international scene. The Department,through the growth path that has been triggered by the MIUR (Italian Ministery of University and Research) Excellence Grant, intends to significantly improve its ranking among the departmental mathematical structures, by facing complex interdisciplinary issues in which it believes it is able to achieve leadership positions at an international level. To this end, the Department has prepared a scientific project, illustrated below, which is organized around the paradigm

modelling, simulation, prediction, control

since it believes that, through this paradigm, Mathematical Sciences can play a decisive role in the development of the future world.

The planned activities, together with new human resources, will lead to a significant breakdown of disciplinary barriers, thus increasing the transversal nature and the breath of research. The researchers involved in our activities will be induced to participate in a greater number of competitive projects and/or collaborations with non-academic partners. The significant increase in the number of doctoral, post-doctoral and researcher positions will produce a critical mass of young scientists; this will offer concrete job opportunities, not only to bright Italians, but also to talented foreign scientists, who might be attracted by a series of available benefits. A significant strengthening of training activities at the Master and Doctoral levels will have a beneficial effect not only on the overall growth of knowledge, but also on the creation of generations of young talents, who will be better prepared to operate successfully in the future socio-economic context.

The scientific project

Starting from the awareness of the role currently played by mathematical models in the very diversified scientific, technological, economic and social environments, the synergetic effort of the Department's researchers will have the aim of attaining higher levels of complexity than the current ones, in the definition, validation, analysis, implementation and application of innovative mathematical models of various nature. In order to reach such an ambitious goal, the Department intends to exploit its internal know-how in an integrated way, hire new top scientists from around the world, and benefit from the multi- and inter-disciplinary environment of the Polytechnical School it is part of. One of the strengths of the project, at the training level, is the presence of both the Master Degree Programme in Mathematical Engineering, established within the Department, which, for several years now has represented a clear reference on the Italian Applied Mathematics scene, and the Inter-University Doctoral Programme in Pure and Applied Mathematics, carried out under an agreement with the University of Turin; both the Master Degree and the Doctoral Programmes, after being appropriately reinforced, will contribute to creating a new generation of young researchers focused on the various themes of the project. The advanced research and training activities connected to the project will require certain specific

actions at the infrastructural level, which, overall will create a more favourable environment for scientific interactions in the Department; this will include the establishment of a new laboratory, equipped with advanced hardware and software, devoted to simulation activities.

One of the most distinctive and original feature of this project is the strong focus on the mathematics of complex networks. In all the problems that we consider, networks appear either as primary research objects or as natural and useful modelling tools. Networks can be used to model infrastructural systems, social and economic relationships, protein interaction schemes, underground fracture architectures, or chemical reaction systems. In the mathematics of complex networks, deterministic and random formalism often coexist, and their tuning and reliable use typically pose significant big data statistical problems. The presence of time and space multi-scales, as well as the simultaneous presence of heterogeneous geometrical objects are other relevant features of these models. Their investigation calls for a sophisticated combination of different mathematical tools. The analysis of models, composed of hierarchical layers of sub-models and sub-structures, represents one of the main scientific challenges of this project.

It is important to stress that a highly interdisciplinary approach will be adopted to reach the general goals of the project, in which the mathematics of a more theoretical nature, applied and computational mathematics, and mathematical statistics will contribute, in an integrated manner, to designing the new tools that are needed to realize the paradigm of *modelling, simulation, prediction, control* in a wealth of different situations. Such an approach, extended to the whole department, certainly represents an innovative aspect in the national mathematical environment; it allows the kind of knowledge integration that is found in the world's most advanced research centres to be attained. The following Institutes are examples of such centres, which we consider valid international benchmarks:

IDSS-MIT, Boston https://idss.mit.edu
AICES-RWTH, Aachen https://www.aices.rwth-aachen.de/en/home
CMMB, Nottingham http://www.nottingham.ac.uk/cmmb/

The structure of the project

The departmental scientific project is structured in four, mutually interconnected, main themes. They are:

T1. *Resilient control for network systems*

T2. *Nested mathematical models in biomedicine*

T3. *Numerical methods for models with high geometric complexity*

T4. *Approximation and statistical inference in random reaction (and interaction) networks*

The description of the four main themes

The scientific motivations that underlie each main theme are provided hereafter, and the research topics that will be the subject of specific investigation within the theme are described.

Theme T1. Resilient control for network systems

The ability to predict and optimise the behaviour of complex socio-technical systems is one of this century's main scientific themes. It is becoming clearer and clearer how the behaviour of large-scale infrastructural, social, economic and financial networks can have a huge societal impact, e.g., enabling or limiting access to essential services, such as mobility and energy, influencing the outcome of elections, or destabilizing entire economies. A central aspect of such network systems is the role played by interconnections in amplifying and propagating shocks through cascading mechanisms that may increase the fragility of a system [8, 24, 1]. The term "systemic risk" refers to the possibility that even small shocks localized in a limited part of the network can propagate and amplify through cascading mechanisms, thus possibly achieving a significant global impact [50, 3]. Resilience is the ability of a system to absorb the largest possible set of shocks, thus avoiding or limiting their propagation on a global scale, and maintaining adequate performance levels [43].

One of the greatest challenges for the mathematical theory of control systems is to create solid scientific foundations and computationally efficient methodologies for the analysis of systemic risk and the design of resilient network systems [42]. During the last couple of decades, static notions of resilience have been proposed, mainly related to network connectivity. The much more ambitious objective is to develop novel dynamical notions of resilience that, on the basis of the system's nature and the structure of its interconnections, would enable its level of systemic risk to be characterised and the control strategies that could increase its resilience to be synthesised.

Within this MIUR Excellence Project, the Department of Mathematical Sciences will concentrate a great deal of research efforts on the development of mathematical models and tools for the analysis of systemic risk and the resilient control synthesis of network systems. This contribution will be of a foundational and methodological nature, with three main application domains: social networks, infrastructure networks (such as transport and energy) and economic and financial networks. Some promising results achieved in this direction include [35, 36, 2, 33, 34].

The first phase of this Project will concern the development of proper notions of network centrality, which will allow the effects that local perturbations can have on a complex interconnected system to be analysed and estimated, and hence its level of resilience to be assessed. In the second phase, more complex models, in which the coupling between the nonlinear interactions and the network topology can induce synchronization effects and cascading mechanisms that could potentially achieve significant systemic effects, will be considered. The final phase will concern the design of decentralized and distributed feedback controls and their implementability, with particular focus on the coupling between information flows and physical system dynamics. In this phase, it will be crucial to validate the considered models on real datasets, including those obtained in collaboration with other research centres and companies, in both Italy and abroad.

Various mathematical techniques, from both discrete and continuous mathematics, including

the graph theory, game theory, functional analysis, optimization, control systems, etc., will be used to model network dynamics. In many cases, nonlinear network dynamics will play a key role in these systems, and will require non-trivial adaptations to networks of classical theories and results. More sophisticated theories, such as random graphs, percolation, quantic graphs, [4, 5, 6], and so on, will prove useful to obtain deeper results.

Because of the interdisciplinary nature of the proposed research topics, the Project will benefit from undergoing collaborations with economists and control theorists, such as D. Acemoglu (MIT), F. Bullo (UCSB), M. Dahleh (MIT) and F. Vega Redondo (Bocconi).

Theme T2. Nested mathematical models in biomedicine

In biology and medicine, each and every macroscopic phenomenon is intrinsically related to small-scale dynamics at a microscopic level. In fact, the collective behaviour of cell aggregates is dictated by the activity of a single cell, which in turn is determined by the inner dynamics of the cell: the over- and under-expression of proteins develop thanks to the activation of the protein networks. The branches of such interaction networks are characterised by feedback mechanisms that link the proteins that are ideally located in the nodes of the network through promotion-inhibition mechanisms.

The mathematical models that deal with biological systems should therefore incorporate phenomena that occur at different space and time scales (see for example [66]); this makes the mathematical problems intrinsically multi-scale (or multi-level). It is in fact necessary to consider processes that occur at the tissue scale (usually represented by continuum mechanics models and mathematically characterized by systems of partial differential equations), at the cellular scale (usually described by kinetic e individual-based models [12, 69]), and eventually at the sub-cellular scale (typically described by systems of ordinary differential equations [19]).

The first modelling goal of the project is that of determining the relationship between the parameters that appear in the macroscopic and mesoscopic models with the output of the microscopic models that describe the subcellular dynamics of the protein networks. The second goal is that of interfacing mathematical models that naturally resolve different spatial scales. In fact, the way of describing a biological phenomenon is not unequivocal, and each approach offers advantages and disadvantages, in terms, for example, of the balance between the accuracy of the description and its computational cost. Fortunately, it is not always necessary to maintain the same level of detail in many applications. The intention is therefore to use mathematical models as a kind of virtual microscope [61, 41], and to only resolve cell and sub-cell levels when absolutely necessary, and to be less focused when a more detailed, yet computationally expensive description is not necessary.

The first step to interface models that operate at different spatial scales is to re-interpret the results obtained for the same biological phenomena but with different models. This up-scaling process will allow modelling parameters that cannot immediately be linked to be inter-related. In the same vein, a fundamental step is to ensure the conservation of the mechanical quantities when passing from a microscopic to a macroscopic model, and vice versa. This process will link the cellular and sub-cellular mechanical parameters to those that constitutively characterize the tissue through virtual rheological experiments performed on cell aggregates,which will be

represented by individual-based models.

It is also important to offer a solid theoretical basis for the interfacing of the hybrid and multiscale models, also in consideration of their rigorous numerical treatment. In this context, we will study the application of various analytical methods – such as formal homogenization [21], different definitions of convergence in a variational setting [59], "mass transportation" techniques [40] – to the analysis of the mathematical properties of the above mentioned models.

Several international collaborations are already active on these themes; among others, mention can be made of the joint work with M. Chaplain (S. Andrews), J.A. Carrillo (Imperial College) and P. Friedl (MD Anderson Cancer Center).

Theme T3. Numerical methods for models with high geometric complexity

The increasing availability of computational resources has allowed mathematical models to be enriched and simulation scales to be enlarged. In the case of complex models, obtained by combining sub-models of a different nature, such as, for example, the ones indicated in the Theme T2, a relevant issue is the need to create interfaces between different numerical methodologies in order to optimize the use of computational resources.

In numerical modelling, one of the sources of persistent complexity is the presence of dimensionally inhomogeneous geometric objects. Let us consider for example: objects obtained through the deposition of homogeneous materials in which fibres are immersed to provide the material with an increased directional strength property [62, 63]; strongly fractured media, in which the flow (fluid, heat or pollutants) mainly occurs within the fractures, but where the surrounding matrix does not have a completely negligible contribution [7]; medical contexts, where it is necessary to simulate the transport of medicines through the circulatory system, up to specific tissues, through extremely confined structures [53]; biological applications, such as those considered in the T2 section, where the fibrous structure of the extra-cellular matrix influences the mechanical and functional properties of biological tissues and, at the smallest scale, the migratory characteristics of tumour cells and the behaviour of the immune system [51].

In the previous topics and in many other contexts, geometrical sub-structures play a fundamental role in the simulation process, but their numerical treatment, due to geometrical constraints, may require a (finite element, or finite volume) mesh with elements at a much smaller scale than the mesh scale required for the model. In fact, a standard approach would lead to the introduction of an unacceptable quantity of numerical unknowns, and would place very serious limitations on the mesh generation process, in order to respect the conformity of sub-structures. For this reason, constrained optimization techniques have recently been applied successfully [14, 16] to the discretization of some models containing geometric inhomogeneities in a less binding and more easily applicable way. The project will develop these techniques and extend their application to new and wider contexts: in the medical field, in the case of the coupling of problems in capillaries with problems in the surrounding tissues, or in order to simulate the propagation of neuron networks; or in situations where the anisotropy of the materials and the presence of reinforcing fibres endow the materials with special characteristics. The project also aims at investigating the possibility of simulating fracture propagation using a Gamma-convergence modelling approach [23].

The achievement of a high level of robustness in the simulation process will constitute the required starting point for the implementation of uncertainty quantification procedures; this will be achieved through stochastic analyses in the presence of a strong randomness about the geometrical configurations or about the characteristics of the materials [13, 15]. In this context, with reference to the Theme T4, it will be important to develop numerical models that incorporate appropriate methods from the data assimilation field.

The objectives outlined above will also require a more detailed study of various complementary research lines: the study of adaptive methods that automatically recognize numerical error sources and adapt the allocation of computational resources according to the specific structure of the phenomenon that has to be simulated [26, 27]; the study of the coupling of finite elements and boundary elements for the treatment of evolutionary models in arbitrary geometries [47, 48, 46]; the study of appropriate Gabor frames and wavelets [37, 39] adapted to the geometry of the problem in the phase space, in order to reduce the complexity of the models through scattered representations of partial differential equations and, more in general, of operators [25, 38], with applications in the quantum mechanics field and in the analysis and processing of analogic and digital signals.

In order to reach an adequate theoretical understanding of the complex internal structure of the geometrical objects involved in the numerical modelling described in the previous points, it is useful to resort to differential geometry methods. In fact, the fibres or fractures of a material may be interpreted as 1-dimensional sub-varieties (fibres) or 2-dimensional sub-sub-varieties (fractures), possibly singular, immersed in a 3-dimensional manifold (homogeneous material). The mechanical or biological constraints are encoded by means of tensors and tensor fields (for example, stress tensors or curvature tensors) in differential relationships that are satisfied by the curvatures, or other differential invariants, of the sub-varieties, which are therefore highly not generic [52, 22, 31]. However, the classical approach, which is based on analytic or topological-differential methods, is not adequate or even fails for efficient numerical modelling. Therefore, it will be necessary to resort to discrete differential geometry techniques. This is a relatively new field of research, which has the primary objective of designing discretizations, which, at the limit, reproduce the classical model [18]. It is necessary to bear in mind that the rich internal geometrical structure of the involved geometric objects makes the creation of adequate discretizations highly non-trivial. In fact, the discretization must encode the curvatures, the differential operators and the differential relations which are typical of the classical objects, and which are necessary to encode the mechanical constraints. In this direction, the project aims at developing synergies between the applications described in the previous points and basic research in differential geometry. The project also aims at creating advanced skills in the field of discrete differential geometry, which is not yet well represented in Italy.

As mentioned above, the geometric properties and the mechanical or biological constraints can be formalized by means of tensors. These algebraic objects occur in a natural way whenever data cannot be represented by matrices but must be organized in multidimensional arrays, that is, in tensors with three or more indices (for example, the Riemann curvature tensor). An interesting and challenging problem of great interest is the study of efficient algorithms for the decomposition and reduction, in canonical form, of tensors. The use of ad hoc decompositions

is crucial both in the theoretical field and in applications, such as in chemistry or in the study of images and time networks (in this direction, numerical calculation algorithms, for example CANDECOMP / PARAFAC, have proved to be extremely useful). The theoretical analysis of the algorithms that underlie these decompositions has a counterpart in algebraic geometry and commutative algebra that has not yet been fully developed, and which will be the subject of investigation in the project [57, 29, 20, 30].

Collaborations are already underway on various aspects of this theme, with R.H. Nochetto (Maryland), S. Sauter (Zurich), K. Groechenig (Vienna), R.L. Bryant (Duke), F. Catanese (Bayreuth University, Germany), E. Hubert (INRIA Mediterranee, France), M. Hegland (ANU, Australia).

Theme T4. Approximation and statistical inference in random reaction (and interaction) networks

Several phenomena in systems biology (cf. also the Theme T2), finance, economy and social sciences (cf. also the Theme T1), telecommunications and industrial production can be modelled as interconnected Markov Chains [10, 70, 32, 68]. In the specific languages of the different application, they are described as reaction networks, Petri nets, random graphs, interacting particle systems, but they all share a common mathematical ground based on the theory of stochastic processes. In such a context, we propose two main research directions: the development of approximated models and their calibration with experimental data. The complexity of such models is due to the large number of agents, which may render them impractical. Several approximation methods have been developed to reduce this complexity, e.g. the fluid limit [55] (when the number of agents becomes very large, the system converges to the solution of an ode system), or the diffusive approximation [56]. However in many practical applications the classical results are not effective. A key goal of this project is to develop new approximation methods, and clarify and enhance the applicability of the classical ones. A first example of interest is that of Markov models with a bounded state space, where the diffusion approximations are only applicable up to the first crossing time of the boundary [58, 11]. Moreover, while the known approximations are valid up to a finite time horizon, it is still not clear whether, and under what conditions, they can be extended to cover the long time behaviour [28, 9]: we also aim to achieve a better understanding of the conditions which will allow the limits in the number of agents, as well as in the amplitude of the noise and time, to be exchanged [49]. Another case where classical approximation results are not applicable is that of nested subsystems (cf. the Theme T2) that interact either on a network that is not complete [54, 60] or at different scales. Such multi-scale or hybrid phenomena are frequent in applications. Classical approximations may often only be applied to some subsystems, and controlling the quality of the overall approximation error, e.g on families of random graphs [34], is a further goal of the project. Further topics that we aim at addressing are the persistence of some properties of the network (e.g. the Markov property) under decimation of the nodes [67, 44], and the problem of multi stability of reaction networks [65].

The second main direction of research within the present Theme consists of statistical methodologies to tune stochastic models (as those described above) in order to match them with exper-

imental data. For such a model, it is of paramount importance to be able to extract information from both the mean behaviour and the noise. The latter may in fact contain information on certain parameters of the system that could be overlooked if naive methodologies were adopted. This problem is not simple, since the likelihood is almost never explicitly known, and even when it is known, it is often numerically intractable. We aim at both applying the most recent techniques in new domains (cf. the book [70] for a review), and at developing new methodologies for parametric inference (cf. [17]) and model verification. Furthermore, we intend considering real applications on experimental data from systems biology, chemistry, pharmacokinetics, pharmacodynamics, as well as disease modelling in clinical and pre-clinical trials [45]. A last goal is that of applying model-free machine learning tools, such as Topological Data Analysis (TDA), to work alongside model-based classical statistical inference. The motivations for the use of these new methodologies arise from their independence of the chosen coordinate system, and their ability to work simultaneously at different scales, thus allowing for multi-scale analysis at a mesoscopic level (cf. the Theme T2 and [64]). Although, on the one hand, TDA allows the complex networks approach to be broadened (cf. the Theme T1) by multi-body interactions, on the other hand, it also allows the notion of *shape* to be added to the description obtained by classical methodologies.

Among the collaborations already in place on such a topic, we highlight those with S. Ditlevsen (Copenhagen) and D. Nutt (Imperial College)

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