Preface

This Proceedings book contains selected papers of the Speakers of the 6th Ph.D. Summer School/Conference on "Mathematical Modeling of Complex Systems" , which took place at the University "Gabriele d'Annunzio" of Chieti-Pescara, 3–11 July, 2019. This was the latest in a series of events, which started at the University of Patras, Greece, in July 2011, organized by Professor Tassos Bountis, whose second realization occurred one year later at the University "Gabriele d'Annunzio" of Chieti-Pescara, in July 2012. These Summer Schools then continued annually, with the 3rd one taking place at Heraklion, Crete, the 4th in Athens, and the 5th one in Patras, Greece, July 2015. Thus, we arrived at the 6th realization of this series of events, in July 2019 at the University "Gabriele d'Annunzio" of Chieti-Pescara https://www.sci.unich.it/mmcs2019/.

The main aim of these Schools is to bring important researchers and teachers, working in various fields of Nonlinear Science and Complexity, to give introductory lectures but also present their recent results to postgraduate or advanced undergraduate students and young researchers from European countries, but also from other countries around the world. They last approximately 8-9 days and, besides their educational and scientific content, also include an introduction of the participants to cultural and recreational centers of the locations where the Schools take place. Thus, in Pescara, the participants had the opportunity to explore interesting cultural sites of the city, visit the University of Chieti-Pescara, and spend their free time at nearby resort towns, enjoying the sea and Italian culinary delicacies!

Most importantly, the 6th Ph.D. Summer School/Conference was dedicated to the memory of Professor Gregoire Nicolis, of the Universite Libre de Bruxelles, who recently passed away. Professor Nicolis, as one of the founding fathers and most influential advocates of Complexity Science, was an invited speaker in the Conference on "Nonlinear Science and Complexity" at Pescara, July 2009. Gregoire Nicolis (1939–2018) was born in Greece and obtained his undergraduate diploma in engineering from the Technical University in Athens. He received his PhD from Ilya Prigogine (Nobel laureate of Chemistry, 1977) at the Free University of Brussels (ULB) in 1965, on "Some Aspects of Transport Phenomena in Nonuniform Systems", and later became Professor and Director of the Center for Nonlinear Phenomena and Complex Systems" (CENOLI) at ULB. He first became known for his work on the development of the theory of dissipative structures in irreversible thermodynamics, while in the last 3 decades evolved into a principal leader in the field of Complexity, on which he wrote many seminal papers as well as important educational volumes. In 1970 he received the Prix Theophile de Donder from the Royal Belgian Academy of Sciences, of which he was a member since 1976. He also was a member of the Academia Europaea and a corresponding member of the Academy of Athens. He was co-editor of the Journal of Nonequilibrium Thermodynamics, the Journal of Statistical Physics, and several other journals in the fields of Chemical Physics, Dynamics and Stability, as well as Bifurcation and Chaos. Nonlinear phenomena and complex systems have become very important scientific fields, since the middle of last century, aiming to understand and solve fundamental problems in many scientific fields that share common features, by the use of mathematical methods and models. The particular focus of the 6th Ph.D. School/Conference was on the connections between Information Theory and Complexity through the relevant role of Entropy. In the study of Complex Systems, probability distributions represent a fundamental tool. Indeed it is known that in physics the equilibrium state of a multi-component system is described by an entropic form constrained by a given observable as for example the internal energy. This entropic form can be obtained as an optimization problem, based on the outcomes of an observable corresponding for instance to the available energy levels. From a thermodynamical point of view, after the pioneering work of Ruppeiner, who introduced a Riemannian metric in the thermodynamical parameter space starting from potentials like entropy and free energy, a rich literature has been developed to analyze the implications that geometry might have on thermostatistics, and perhaps also thermodynamics. In recent years, there has been a growing interest in the study of statistical physics by means of Information Geometry. In this framework, the methods of differential geometry are applied to deduce properties of statistical manifolds, generated by parametric families of probability distribution functions. Information Geometry investigates the geometric structures of the statistical manifolds, introducing first a Riemannian metric derived from Fisher's information matrix (Fisher–Rao metric). Many efforts have been devoted to better understand the role of geometry in statistics. For example, Cencov proved that the Fisher–Rao metric is the unique metric, monotone under the trasformations of the statistical model, that implies the uniqueness of the induced affine connection in a statistical manifold. Csizsar defined the concept of f-divergence, Efron studied the role of curvature in a statistical model as a quantification of the information, while Eguchi related the affine connection to a divergence function or relative entropy. More recently, Amari showed the existence of a rich geometry in the probability space. More precisely, he introduced a couple of affine connections dually flat with respect to the Fisher–Rao metric, the so called alpha-connections, which have fundamental importance in estimation theory.

Information Geometry has a long tradition in Pescara. Indeed, the first Conference on "Information Geometry and its Applications" was organized here in July 2002 with the presence of its "historical father", Professor Shun'ichi Amari from University of Tokyo. Another founding father, who was present at that time and also came to the 6th Summer School in Pescara, Professor Giovanni Pistone, spoke on possible extensions of the geometric structure on the space of probability measures in the infinite dimensional case.

As one of the most famous experts in the world on the subject of Entropy, Professor Constantino Tsallis was present in the 6th Summer School to speak about his work on non-extensive thermodynamics. Furthermore, other important applications of Complex Systems were discussed in the School, such as those in Biomedicine and Neuroscience, where very important lectures were given, among others, by Professor Athanassios Fokas from Cambridge University.

This volume of Proceedings is organized in the following way.

The first paper is a collection of main topics of Complexity Science, based on the ideas of the late Professor Gregoire Nicolis and written by Vasileios Basios and Stamatios Nicolis, Gregoire's son. Precisely, in the paper "Gregoire Nicolis, one of the founders of Complexity Science: a recollection", the authors eloquently describe the main reasons why the late Professor G. Nicolis has had, through his many papers and books, significant influence first on the development of modern statistical mechanics, physical chemistry and nonlinear dynamics. The authors then concentrate on the last 3 decades of his life and emphasize his contribution to founding the field of Complexity (or Complex Systems Science), which has gained so much popularity and prominence in our times. In particular, the authors, after reviewing the central ideas of his many contributions, discuss two specific and currently expanding areas of research that are an important part of his rich heritage: The first originated from his work on a new paradigm of crystallization and aggregation, and is in fact related to the currently very exciting field of self-organized, adaptive or 'smart' materials. The second is, of course, his pioneering ideas on the interdisciplinarity of complex systems, which, within the framework of biology, are currently leading the investigation of coordinated motion and decision making in collective dynamics of social animals.

An interpretation of certain complex topics arising in Genetics was presented and discussed in A. Athanassiadou's paper (The genetic complexity of the human genome in health and disease: basic concepts). It gives an informative account of the determination of the human genome, describes the complex methods and approaches used to study the molecular basis of genetic structures and processes, and offers an up-to-date account of our understanding of the subject. More precisely, the paper focuses on the different levels of complexity in the human genome: The first level refers to the expression of protein coding genes, as regulated by their individual promoter in linear proximity. The next level of genetic complexity involves long distance action by far away enhancers, interacting with promoters through DNA looping. This 3-dimensional regulation is further developed by chromosome folding into the so-called transcription factories, for full physiological expression. Chromosome folding, mediated by specific genetic elements - insulators, further adds to the genetic complexity. The relevance of this research for Precision Medicine and, more generally, Genomic Medicine in treating a variety of diseases is explained.

Regarding Complexity in Medical Sciences, several talks with applications in Imaging and Dentistry were also presented at the 6th School.

More precisely, in the paper by N. W. Falasca and R. Franciotti (The ability of Granger causality analysis to detect indirect links: a simulation study) Granger causality is considered. Usually it is a way to investigate causality between two variables in a time series, mostly applied in Econometry. The method is a probabilistic account of causality which uses empirical data sets to find patterns of correlation. In this work, the authors investigate if Granger causality can distinguish between direct and indirect influences, performing the analysis on simulated electroencephalographic cerebral signals.

A. Pasculli, F. Rizzo, M. Mangifesta, and A. Viskovic (Modeling of crew-dental structure interaction. First step toward finite element analysis) detect the fracture mechanism that occurs during the screw penetration in the support and during the structure vibration in dental implants. In order to study a methodology that minimizes the local damage of the dental material, due to the generation of micro-cracks following the implantation actions, numerical analyses by Finite Element Method (FEM) are calibrated through experimental laboratory measurements on different support materials and screws typologies. Uncertainty due to the laboratory error propagation is investigated using Polynomial Chaos Expansion (PCE) of experimental measurements.

As last medical application, V. Perrotti, G. Iezzi, and A. Piattelli (Correlation between bone density and fractal dimension: a pilot study) use fractal analysis to describe the complex internal architecture of bone tissue. Their aim is to detect whether the fractal dimension (FD) is able to distinguish between different trabecular bone densities (BD), assessed histo-morphometrically, in order to support the use of FD as a supplementary method, which is non-invasive because it can be measured on radiographs (periapical, digital panoramic images, cone beam computed tomography), to investigate BD measurement during healing, inflammatory processes and pathologies associated to bone breakdown.

Additional aspects of Complexity in physical systems were presented by Tassos Bountis, Constantino Tsallis, Haris Skokos, Marko Robnik and others, whose contributions are included in this volume and separately discussed below.

Anastasios Bountis (Complex dynamics and statistics of 1-dimensional (1-D) Hamiltonian lattices: long range interactions and supratransmission) offers in his paper an extended introduction to the dynamics of Hamiltonian systems, aiming to explore the dynamical and statistical properties of 1-D nonlinear Hamiltonian lattices of N coupled oscillators. After explaining the methods of GALI, he applies them to these lattices to identify regular motion on invariant tori from that of chaotic regions. Furthermore, he distinguishes between weak and strong chaos, connecting the former to stickiness effects in phase space, showing that typically their statistical properties are not described by the Gaussian distributions, but rather by the so-called q-Gaussian, introduced by Tsallis. Then he extensively analyzes the degree of chaos and its transport properties in the case of short-range interactions (SRI) as opposed to the long-range power-law interactions (LRI). The transition from stronger to weaker chaos in terms of the maximal Lyapunov exponents is demonstrated by increasing the strength of LRI and also the number N of particles/oscillators in the chain. Finally, he examines the fascinating property of supratransmission, which occurs through an external harmonic driving on a boundary particle. When the amplitude of driving exceeds a certain critical value the energy can be transported along the chain in the form of a nonlinear wave without being trapped in some finite part of the lattice. The author describes his recent work, and that of his collaborators, on these complex phenomena and points out some of their surprising aspects, which have yet to be analytically understood.

In their paper "Extensive numerical results for integrable case of standard map", Ugur Tirnakli and Constantino Tsallis, first note the fact that in the past few decades conservative dynamical systems, i.e. ones that conserve "volumes" in phase space, have become a very important area of research not only from a dynamical, but also from the a statistical mechanical viewpoint. In particular, much work has been devoted to a simpler but quite representative class of examples described by conservative discrete dynamical systems or maps. Tirnakli and Tsallis then concentrate on one of the most familiar paradigms of such a system defined in 2 dimensions by the area-preserving Chirikov–Taylor map, more widely known as the standard map, containing a single nonlinearity parameter $K \neq 0$. The authors briefly review their recent work on the statistical analysis of this map (in the spirit of the Central Limit Theorem), where they have numerically shown that the probability distribution function (pdf) of the sum of the suitable random variable is well approximated by a Gaussian, when the initial conditions are randomly selected from the chaotic sea. However, when initial conditions are chosen from within a "regular region" (stability islands) the pdfs are q-Gaussian! Remarkably, the same q-Gaussian (and with the same q value!) is obtained, even in the limit of the linear (integrable) case of $K = 0$! The authors emphasize that this is quite a remarkable result for which there is still no analytical explanation available.

In their paper (On the behavior of the Generalized Alignment Index (GALI) method for regular motion in multidimensional Hamiltonian systems) Henok Moges, Thanos Manos, and Charalampos Skokos investigate the behavior of the Generalized Alignment Index of order k (GALIk) for regular orbits of multidimensional Hamiltonian systems. Prof. Skokos, who was present in Pescara, is well – known for his work on efficient chaos indicators over the past 20 years. He has played a crucial role in inventing the GALI method and applying it in a great variety of conservative systems. In this paper, he and his co–workers focus on the study of regular orbits in the neighborhood of two typical, stable periodic orbits of the Fermi-Pasta-Ulam-Tsingou (FPUT) model, in $N = 11$ degrees of freedom, and show that the asymptotic GALIk values decrease when the energy approaches the destabilization of the periodic orbit, while they increase when the considered regular orbit moves further away from the periodic one for a fixed energy. Furthermore, the asymptotic GALIs of higher order attain lower values, while the GALIk values increase as the distance from the island's boundary grows, while as one approaches the destabilization energy of the SPO the GALIk values decrease. In addition, by performing extensive numerical simulations, the authors show that the index's behavior does not depend on the choice of the initial deviation vectors needed for its evaluation.

Next, in the paper (Properties of normal modes in a modified disordered Klein–Gordon lattice: from disorder to order) the authors B. Senyange, J.-J. du Plessis, B. Many Manda, and Ch. Skokos introduce a linear version of the disordered Klein–Gordon (DKG) lattice model, whose potential includes quadratic nearest — neighbor particle interactions as well as onsite terms whose harmonic term has randomly varying coefficients. Their model possesses two parameters that can be used to control the disorder strength. They are D, which determines the range of the coefficients of the on-site potentials, and W, which defines the strength of the nearest-neighbor interactions. They fix

$W = 4$ and investigate how the properties of the system's normal modes change as one approaches order, i.e. $D > 0$. They show that the probability density distribution of the normal mode frequencies tends to a 'U'-shaped profile as D decreases. Furthermore, to estimate the modes' spatial extent they use two quantities, the so-called localization volume V (related to the modes' second moment) and the participation number P. They show that both quantities scale as $\propto D^{-2}$ when D approaches zero and they numerically verify a proportionality relation between them as $V/P \approx 2.6$. Now, as is well - known, the nonlinear DKG Hamiltonian is a physically relevant system that can model atomic arrays subject to external fields, e.g. anharmonic lattice vibrations in crystals. Thus, the authors' analysis here constitutes a first step towards understanding in more depth the influence of disorder on the chaotic behavior of the DKG system.

The paper by Marko Robnik (A brief introduction to stationary quantum chaos in generic systems) provides a comprehensive and clear overview of a very interesting and far-reaching scientific field, named quantum chaos (or wave chaos), in which the author has played a major role. This field was born almost 40 years ago to demonstrate that the concepts of chaos are not limited to classical physics, but have also an important counterpart in the quantum world. In this paper, the author eloquently reviews the basic aspects of quantum chaos in Hamiltonian systems whose classical phase space contains regular regions that coexist with chaotic regions. He points out that the quantum evolution of classically chaotic bound systems is based on the (linear) Schrodinger equation and hence no chaotic behaviour can occur, as the motion is always almost periodic. However, the stationary solutions of this equation in the quantum phase space reveal a precise analogy between quantum observables and the structure of the classical phase portrait. The author proceeds to describe this analogy in detail in terms of spectral (energy) statistics and random matrix theory. Of particular importance is his identification of the classically mixed phase space with quantum energy level statistics described by the Berry–Robnik distribution. The author also emphasizes the crucial role of the Heisenberg time scale $t_H = 2\pi h/\Delta E$ in quantum systems with discrete energy spectrum (ΔE is the mean level spacing) and its relation to the classical transport time scale t_T. Indeed it is their ratio that determines the degree of localization of the chaotic eigenstates. Finally, the author discusses the structure of quantum localized chaotic eigenstates in connection with the distribution of localization measures and shows that the localized chaotic states display a fractional power-law repulsion between nearest energy levels, as demonstrated in the examples of a quantum kicked rotator, the stadium billiard, and a mixed-type billiard.

In the paper by B. Rahman (Time-delay systems: a review), the author gives an informative account of the time-delay systems by first showing a simple example, and then by defining general and different versions of time-delay, namely a discrete (single or multiple) time-delay, the distributed (the evolution depends on the entire history of the process, but with different weights described by the probability density distribution) and the combination of both. One important feature of time-delay systems is that the oscillations and chaotic motion can be suppressed. This mathematical modeling is motivated by real applications in many systems, like physiological, biological, social, physical and engineering problems. Neural networks are perhaps the most prominent example. The next level of complexity arises when the variation in time of the time-delay must be taken into account, especially in biological and social systems, in contrast to e.g. the optical systems where little variation is observed and needed. The paper offers a list of useful up-to-date references on the subject.

In their paper "A primer on Laplacian dynamics in directed graphs", J. J. P. Veerman and R. Lyons review in a brief but comprehensive way some fundamental properties of the theory of directed graphs (or digraphs as they are called). In particular, they discuss the solutions of the differential equations $dx/dt = -Lx$ and $dp/dt = -pL$, where x and p designate the location of digraph points, and L is the "Laplacian" matrix having some specific properties mentioned in the text. The authors explain that these equations describe the dual processes of "discussion" and "consensus" respectively, and develop in their paper the theory leading to their asymptotic behavior as $t \to \infty$, where the time variable t can be continuous or discrete. Next, they apply this theory to the “random walk"Laplacian and mention that digraphs constitute a generalization of undirected graphs and thus have many applications, which include the internet, social networks, food webs, epidemics, chemical reaction networks, databases, communication networks and control theory.

An application of Complex Networks and Graph Theory to Finance was considered by M. Eboli (Linearities, non-linearities and phase transitions in loss diffusion processes in financial networks), due to banks and financial institutions are linked by financial obligations that form complex networks. Formally, a financial network is represented by a weighted and directed graph, in which the nodes are financial operators (banks and other intermediaries), and the links are the financial obligations that connect pairs of such operators. These financial networks become the vehicles of financial contagion in the event of liquidity and insolvency shocks. Numerical simulations of recent contagion processes in financial networks are presented in this work, which show unexpected linearities.

D. P. K. Ghikas (From Complexity to Information Geometry and beyond ...) proposes a framework, similar to the three level scheme of physical theories (observations/experiments, phenomenology, microscopic interactions) for the definition and classification of complex systems. As a useful phenomenological modeling for these aims, the author uses some quantities of Information Geometry derived from generalized entropies. Furthermore, to describe the microscopic structure and interactions of the parts, he suggests an algebraic framework for complex systems based on hyper-networks and super graphs, which is also able to offer concrete techniques for calculation.

A short course on Information Geometry of the probability simplex was presented by Giovanni Pistone (Information Geometry of the probability simplex: a short course) and is included in this volume. A statistical model is a parametrised set of probability distributions. The point of view of Information Geometry (IG) is that a statistical model must be viewed as a submanifold of a manifold on all probability distributions. As a geometry of Chance, the language of IG is the language of differential geometry. Non-parametric presentations of differential geometry can be found in the literature, where the model space (coordinates space) can be any Banach space and different charts of the atlas are not required to have the same image space. In this short course, the approach is rigorously non-parametric but the originality is that the author follows the ideas of classical statistical mechanics (Boltzmann–Gibbs theory) which considers the probability distributions as primitive objects with an own intrinsic geometry. From this we deduce the importance of the exponential form, which in turn depends on the hypothesis of strict positivity. The tangent space is the energy space, connected with the transformation in the logarithmic scale of the probability densities which produces entropies as in the physics interpretation. The notion of statistical bundle allows to consider, in a natural way, Fisher information as a intern product of fibres, also to introduce two affine transports, dual each other, and an affine system of chartes, which is intrinsic to the structure. From the related parallel transport, covariant derivatives are deduced. All the construction is generalized to the case of deformations with respect to Tsallis–Kaniadakis–Naudts interpretation.

As a specific application, A. De Sanctis and S. A. Gattone (Information Geometry tools for Shape Analysis) investigate the use of Information Geometry tools in Shape Analysis. Shape Analysis is of interest in various fields such as morphological-metrics, computer vision and medical imaging. More specifically, usually, experts identify a finite number of points, called landmarks, which are representative of a shape. The authors propose to model landmarks of a complex shape by bivariate Gaussian distributions. For every landmark, the geometric coordinates are means which capture uncertainties that arise in landmark placement due to measurement errors. The variances are invisible coordinates reflecting the natural variability across a population of shapes. Therefore landmarks are points in a statistical manifold, where geodesics, with respect to different Riemannian metrics (Fisher–Rao metric and Wasserstein distance) can be defined. Geodesics are thus considered in the paper both to reconstruct the shape evolution in time as well as to derive shape distances to be used in shape clustering.

In the same context, the paper by F. D. Oikonomou (Using the alpha geodesic distance in shapes K-means clustering) considers geodesics with respect to the alpha connections, which constitute a family of affine connections, among which the only Riemannian metric is the Fisher–Rao metric. The aim is to generalize the methodology of the previous paper for this family of connections. In order to detect if it is possible to optimize the alpha parameter, as a first step in the analysis, three different values of the alpha parameter are used to cluster shapes.

In closing this Introduction, we want to thank the Department of Business Administration and Management of University "Gabriele d'Annunzio" to have hosted the 6th Ph.D. Summer School/Conference and Professor Gianluca Amato for the technological support, in particular to have organized the web site: https://www.sci.unich.it/mmcs2019/

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