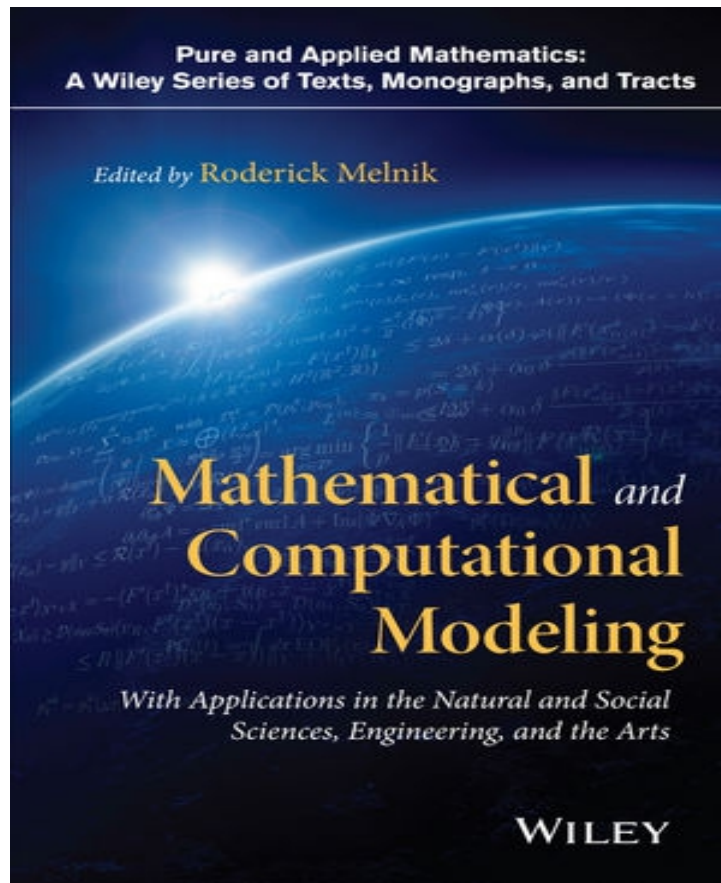# Universality of Mathematical Models in Understanding Nature, Society, and Man-Made World

Roderick Melnik

MATHEMATICAL AND COMPUTATIONAL MODELING

MATHEMATICAL AND COMPUTATIONAL MODELING

With Applications in Natural and Social Sciences, Engineering, and the Arts

Edited by

RODERICK MELNIK
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Teachers who educate children deserve more honor than parents who merely gave birth; for bare life is furnished by the one, the other ensures a good life.
(Aristotle)

To my parents who were my first and most devoted teachers.

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PREFACE

Mathematical and computational modeling has become a major driving force in scientific discovery and innovation, covering an increasing range of diverse application areas in the natural and social sciences, engineering, and the arts. Mathematical models, methods, and algorithms have been ubiquitous in human activities from the ancient times till now. The fundamental role they play in human knowledge, as well as in our well-being, is indisputable, and it continues to grow in its importance.

Significant sources of some of the most urgent and challenging problems the humanity faces today are coming not only from traditional areas of mathematics applications in natural and engineering sciences, but also from life, behavioral, and social sciences. We are witnessing an unprecedented growth of model-based approaches in practically every domain of human activities. This expands further interdisciplinary horizons of mathematical and computational modeling, providing new and strengthening existing links between different disciplines and human activities. Integrative, holistic approaches and systems–science methodologies are required in an increasing number of areas of human endeavor. In its turn, such approaches and methodologies require the development of new state-of-the-art mathematical models and methods.

Given this wide spectrum of applications of mathematical and computational modeling, we have selected five representative areas, grouped in this book into sections. These sections contain 12 selective chapters, written by 25 experts in their respective fields. They open to the reader a broad range of methods and tools important in many applications across different disciplines. The book provides details on state-of-the-art achievements in the development of these methods and tools, as well as their applications. Original results are presented on both fundamental theoretical and applied developments, with many examples emphasizing interdisciplinary nature of

mathematical and computational modeling and universality of models in our better understanding nature, society, and the man-made world.

Aimed at researchers in academia, practitioners, and graduate students, the book promotes interdisciplinary collaborations required to meet the challenges at the interface of different disciplines on the one hand and mathematical and computational modeling on the other. It can serve as a reference on theory and applications of mathematical and computational modeling in diverse areas within the natural and social sciences, engineering, and the arts.

I am thankful to many of my colleagues in North America, Europe, Asia, and Australia whose encouragements were vital for the completion of this project. Special thanks go to the referees of this volume. Their help and suggestions were invaluable. Finally, I am very grateful to the John Wiley & Sons editorial team, and in particular, Susanne Steitz-Filler and Sari Friedman for their highly professional support.

Waterloo, ON, Canada   RODERICK MELNIK
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Universality of Mathematical Models in Understanding Nature, Society, and Man-Made World

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Abstract

An increasing range and diversity of human activities depend critically on the development of new efficient mathematical and computational models, methods, and algorithms. Mathematical modeling methods are now rooted firmly in such diverse areas as earth and climate sciences, nanotechnology and aerospace, social and life sciences, to name just a few. Such methods are becoming a major driving force in scientific discovery and innovation, as well as in shaping model-based predictive capabilities developed by modern science and engineering. In this process, mathematical models demonstrate their universality in our better understanding nature, society, and man-made world. We provide a brief historical account and an overview of these new trends, identify some of the frontier areas for future developments, and give a set of selective examples from natural and social sciences, engineering and the arts.

1   Human knowledge, models and algorithms

There are various statistical and mathematical models of the accumulation of human knowledge. Taking one one them as a starting point, the Anderla model, we would learn that the amount of human knowledge about 40 years ago was 128 times greater than in the year 1 AD. We know also that this has increased drastically over the last four decades. However, most such models are economics-based and account for technological developments only, while there is much more in human knowledge to account for. Human knowledge has always been linked to models. Such models cover a variety of fields of human endeavor, from the arts to agriculture, from the description of natural phenomena to the development of new technologies and to the attempts of better understanding societal issues. From the dawn of human civilization, the development of these models, in one way or another, has always been connected with the development of mathematics. These two processes, the development of models representing the core of human knowledge and the development of mathematics, have always gone hand in hand with each other. From our knowledge in particle physics and spin glasses [4, 6] to life sciences and neuron stars [1, 5, 16], universality of mathematical models has to be seen from this perspective.

Of course, the history of mathematics goes back much deeper in the dawn of civilizations than 1AD mentioned above. We know, for example, that as early as in the 6th-5th millennium BC, people of the Ancient World, including pre-dynastic Sumerians and Egyptians, reflected their geometric-design-based models on their artifacts. People at that time started obtaining insights into the phenomena observed in nature by using quantitative representations, schemes, and figures. Geometry played a fundamental role in the Ancient World.

With civilization settlements and the development of agriculture, the role of mathematics in general, and quantitative approaches in particular, has substantially increased. From the early times of measurements of plots of lands and of the creation of the lunar calendar, the Sumerians and Babylonians, among others, were greatly contributing to the development of mathematics. We know that from those times onwards, mathematics has never been developed in isolation from other disciplines. The cross-fertilization between mathematical sciences and other disciplines is what produces one of the most valuable parts of human knowledge. Indeed, mathematics has a universal language that allows other disciplines to significantly advance their own fields of knowledge, hence contributing to human knowledge as a whole. Among other disciplines, the architecture and the arts have been playing an important role in this process from as far in our history as we can see. Recall that the summation series was the origin of harmonic design. This technique was known in the Ancient Egypt at least since the construction of the Chephren Pyramid of Giza in 2500 BCE (the earliest known is the Pyramid of Djoser, likely constructed between 2630BCE and 2611BCE). The golden ratio and Fibonacci sequence have deep roots in the arts, including music, as well as in the natural sciences. Speaking of mathematics, H. Poincare once mentioned that "it is the unexpected bringing together of diverse parts of our science which brings progress" [11]. However, this is largely true with respect to other sciences as well and, more generally, to all branches of human endeavor. Back to Poincare's time, it was believed that mathematics "confines itself at the same time to philosophy and to physics, and it is for these two neighbors that we work" [11]. Today, the quantitative analysis as an essential tool in the mathematics arsenal, along with associated mathematical, statistical and computational models, advances knowledge in pretty much every domain of human endeavor. The quantitative-analysis-based models are now rooted firmly in the application areas that were only recently (by historical account) considered as non-traditional for conventional mathematics. This includes, but not limited to, life sciences and medicine, user-centered design and soft engineering, new branches of arts, business and economics, social, behavioral, and political sciences.

Recognition of universality of mathematical models in understanding nature, society, and man-made world is of ancient origin too. Already Pythagoras taught that in its deepest sense the reality is mathematical in nature. The origin of quantification of science goes back at least to the time of Pythagoras' teaching that numbers provide a key to the ultimate reality. The Pythagorean tradition is well reflected in the Galileo statement that "the Book of Nature is written in the language of mathematics". Today, we are witnessing the areas of mathematics applications not only growing rapidly in more traditional natural and engineering sciences but also in social and behaviorial sciences as well. It should be noted that the term "universality" is also used in the literature in different, more specific and narrow contexts. For example, in statistical mechanics, universality is the observation that there are properties for a large class of systems that are independent of the dynamical details of the system. A pure mathematical definition of a universal property is usually given based on representations of category theory. Another example is provided by computer science and computability theory where the word "universal" is usually applied to a system which is Turing complete. There is also a universality principle, a system property often modeled by random matrices. These concepts are useful for corresponding mathematical or statistical models and are subject of many articles (see, e.g., [2, 3, 4, 5, 6, 7, 14, 16] and references therein). For example, the authors of [2] discuss universality classes for complex networks with possible applications in social and biological dynamic systems. A universal scaling limit for a class of Ising-type mathematical models is discussed in [6]. The concept of universality of predictions is discussed in [14] within the Bayesian framework. Computing universality is a subject of discussions in [3], while universality in physical and life sciences are discussed in [7] and [5], respectively. Given a brief historical account demonstrating the intrinsic presence of models in human knowledge from the dawn of civilizations, "universality" here is understood in a more general, Aristotle's sense: "To say of what is, that it is not, or of what is not, that it is, is false; while to say of what is, that it is, and of what is not, that it is not, is true". The underlying reason for this universality lies with the fact that models are inherently linked to algorithms. From the ancient times till now,

human activities and practical applications have stimulated the development of model-based algorithms. If we note that abstract areas of mathematics are also based on models, it can be concluded that mathematical algorithms have been at the heart of the development of mathematics itself. The word "algorithm" was derived from Al-Khwarizmi (c. 780 c. 850), a mathematician, astronomer and geographer, whose name was given to him by the place of his birth (Khwarezm or Chorasmia). The word indicated a technique with numerals. Such techniques were present in human activities well before the 9th century, while specific algorithms, mainly stimulated by geometric considerations at that time, were also known. Examples include algorithms for approximating the area of a given circle (known to Babylonians and Indians), an algorithm for calculating π by inscribing and then circumscribing a polygon around a circle (known to Antiphon and Bryson already in the 5th century BC), Euclid's algorithm to determine the greatest common divisor of two integers, and many others. Further development of the subject was closely interwoven with applications and other disciplines. It led to what in the second part of the XXth century was called by E. Wigner as "the unreasonable effectiveness of mathematics in the natural sciences". In addition to traditional areas of natural sciences and engineering, the XXth century saw an ever increasing role of mathematical models in the life and environmental sciences too. This development was based on earlier achievements. Indeed, already during the 300's BC, Aristotle studied the manner in which species evolve to fit their environment. His works served as an important stepping stone in the development of modern evolutionary theories, and his holistic views and teaching that "the whole is more than the sum of its parts" helped the progress of systems science in general and systems biology in particular. A strong growth of genetics and population biology in the XXth century effectively started form the rediscovery of G. Mendel's laws in 1900 (originally published in 1865-1866), and a paramount impetus for this growth to be linked with mathematical models was given by R. A. Fisher's Fundamental Theorem of Natural Selection in 1930. This result was based on a partial differential equation (PDE), expressing the rate of fitness increase for any living organism. Mathematical models in other areas of life sciences were also developing and included A. J. Lotka and V. Volterra's preditor-prey systems (1925-1931), A.A. Malinovsky's models for evolutionary genetics and systems analysis (1935), R. Fisher and A. Kolmogorov equation for gene propagation (1937), A. L. Hodgkin and A. F. Huxley's equations for neural axon membrane potential (1952), to name just a few. New theories, such as self-organization and biological pattern formation, have appeared, demonstrating the powerful cross-fertilization between mathematics and the life sciences (see additional details in [1]). More recently, the ready availability of detailed molecular, functional, and genomic data has led to the unprecedented development of new data-driven mathematical models. As a result, the tools of mathematical modelling and computational experiment are becoming largely important in today's life sciences. The same conclusion applies to environmental, earth, and climate sciences as well. Based on data since 1880, by now we know that global warming has been mostly caused by the man-made world with its emission from the burning of fossil fuels, environmental pollution, and other factors. In moving forward, we will need to solve many challenging environmental problems and the role of mathematical and computational modeling in environmental, earth, and climate sciences will continue to increase [13].

Mathematical models and algorithms have become essential for many professionals in other areas, including sociologists, financial analysts, political scientists, public administration workers and the governments [12], with this list continuing to grow. Our discussion would be incomplete if we do not mention here a deep connection between mathematics and the arts. Ancient civilizations, including Egyptians, Mesopotamians, and Chinese, studied the mathematics of sound, and the Ancient Greeks investigated the expression of musical scales in terms of the ratios of small integers. They considered harmony as a branch of science, known now as musical acoustics. They worked to demonstrate that the mathematical laws of harmonics and rhythms have a fundamental character not only to the understanding of the world but also to human happiness and prosperity. While a myriad of examples of the intrinsic connection between mathematics and the arts are found in the Ancient World, undoubtedly that the Renaissance brought an enriched rebirth of classical ancient world

cultures and mathematical ideas not only for better understanding of nature but also the arts. Indeed, painting three-dimensional scenes on a two-dimensional canvas presents just one example where such a connection was shown to be critical. Not only philosophers, but artists too, were convinced that the whole universe, including the arts, could be explained with geometric and numerical techniques. There are many examples from the Renaissance period where painters were also mathematicians, with Piero della Francesca (c.1415-1492) and Leonardo da Vinci (1452 1519) among them. Nowadays, the arts and mathematics are closely interconnected, continuing to enrich each other. There are many architectural masterpieces and paintings that have been preserved based on the implementation of sophisticated mathematical models. Efficient computer graphics algorithms have brought a new dimension to many branches of the modern arts, while a number of composers have incorporated mathematical ideas into their works (and the golden ratio and Fibonacci numbers are among them). Musical applications of number theory, algebra, and set theory, among other areas of mathematics, are well known.

While algorithms and models have always been central in the development of mathematical sciences, providing an essential links to the applications, their importance has been drastically amplified in the computer age, where the role of mathematical modeling and computational experiment in understanding nature and our world becomes paramount.

2   Looking into the future from a modeling perspective

Although on a historical scale electronic computers belong to a very recent invention of humans, the first computing operations were performed from ancient times by people themselves. From abacus to Napier's Bones, from the Pascaline to the Leibnitz's Stepped Reckoner, from the Babbage's Difference (and then Analytic) Engine to the Hollerith's Desk invention as a precursor to IBM, step by step, we have drastically improved our ability to compute. Today, modern computers allow us to increase productivity in intellectual performance and information processing to a level not seen in the human history before. In its turn, this process leads to a rapid development of new mathematics-based algorithms that are changing the entire landscape of human activities, penetrating to new and unexpected areas. As a result, mathematical modeling expands its interdisciplinary horizons, providing links between different disciplines and human activities. It becomes pervasive across more and more disciplines, while practical needs of human activities and applications, as well as the interface between these disciplines, human activities, mathematics and its applications, stimulate the development of state-of-the-art new methods, approaches, and tools. A special mention in this context deserves such areas as social, behavioral, and life sciences. The ever expanding range of the two-way interaction between mathematical modeling and these disciplines indicates that this interaction is virtually unlimited. Indeed, taking life sciences as an example, the applications of mathematical algorithms, methods, and tools in drug design and delivery, genetic mapping and cell dynamics, neuroscience and bio-nanotechnogy have become ubiquitous. In the meantime, new challenges in these disciplines, such as sequencing macromolecules (including those already present in biological databases), provide an important catalyst for the development of new mathematics, new efficient algorithms and methods [1]. Euclidian, non-Euclidian, and fractal geometries, as well as an intrinsic link between geometry and algebra highlighted by R. Descartes through his coordinate system, have all proved to be very important in these disciplines, while the discovery of what is now known as the Brownian motion by Scottish botanist R. Brown, has revolutionized many branches of mathematics. Game theory and the developments in control and cybernetics were influenced by the developments in social, behavioral, and life sciences, while the growth of systems science has provided one of the fundamentals for the development of systems biology where biological systems are considered in a holistic way [1]. There is a growing understanding that the interactions between different components of a biological system at different scales (e.g., from the

molecular to the systemic level) is critical. Biological systems provide an excellent example of coupled systems and multiscale dynamics. A multiscale spatio-temporal character of most systems in nature, science and engineering is intrinsic, demonstrating complex interplay of its components, well elucidated in the literature (e.g., [8, 13, 9] and references therein). In life sciences, the number of such examples of multiscale coupled systems and associated problems is growing rapidly in many different, albeit often interconnected, areas, e.g.

- Complex biological networks, genomics, cellular systems biology and systems biological approaches in other areas, studies of various organs, their systems and functions;

- Brain dynamics, neuroscience and physiology, developmental biology, evolution and evolutionary dynamics of biological games;

- Immunology problems, epidemiology and infectious diseases, drug development, delivery, and resistance;

- Properties, dynamics, and interactions at various length and time scales in bio-macromolecules, including DNA, RNA, proteins, self-assembly and spatio-temporal pattern formation in biological systems, phase transitions, etc;

Many mathematical and computational modeling tools are ubiquitous. They are universal in a sense that they can be applied in many other areas of human endeavors. Life sciences have a special place when we look into the future developments of mathematical and computational modeling. Indeed, compared to other areas, e.g. those where we study physical or engineering systems, our knowledge of biological systems is quite limited. One of the reasons behind this is biological system complexity, characterized by the fact that most biological systems require dealing with multiscale interactions of their highly heterogeneous parts on different time scales.

In these cases in particular, the process of mathematical and computational modeling becomes frequently a driving source for the development of hierarchies of mathematical models. This helps determine the range of applicability of models. What is especially important is that based on such hierarchies, mathematical models can assist in explaining the behavior of a system under different conditions and the interaction of different system components. Clearly, different models for the same system can involve a range of mathematical structures and can be formalized with various mathematical tools such as equation- or inequality- based models, graphs, logical and game theoretic models, etc. We know by now that the class of the models amenable to analytical treatments, while keeping assumptions realistic, is strikingly tiny, when compared to the general class of mathematical models that are at the forefront of modern science and engineering [10]. As a result, most modern problems are treated numerically, in which case the development of efficient algorithms becomes critical. As soon as such algorithms are implemented on a computer, we can run the model multiple times under varying conditions, helping us to answer outstanding questions quicker and more efficiently, providing us an option to improve the model when necessary. Model-algorithm-implementation is a triad which is at the heart of mathematical modeling and computational experiment. It is a pervasive, powerful, theoretical and practical tool, covering the entire landscape of mathematical applications [10]. This tool will play an increasingly fundamental role in the future as we can carry out mathematical modeling and computational experiment even in those cases when natural experiments are impossible. At the same time, given appropriate validation and verification procedures, we can provide reliable information more quickly and with less expense compared to natural experiments. The two-way interactions between new developments in information technology and mathematical modeling and computational experiment are continuously increasing predictive capabilities and research power of mathematical models.

Looking into the future from a modeling perspective, we should also point out that such predictive capabilities and research power allow us to deal with complex systems that have intrinsically inter-connected (coupled) parts, interacting in non-trivial dynamic manner. In addition to life, behavioral, and social sciences, mentioned earlier, such systems arise in many other areas, including, but not limited to, fusion and energy problems, materials science and chemistry, high energy and nuclear physics, cosmology and astrophysics, earth, climate, environmental, and sustainability sciences.

In addition to the development of new models and efficient algorithms, the success of predictive mathematical modeling in applications is dependent also on further advances in information sciences, and the development of statistical, probabilistic and uncertainty quantification methods. Uncertainty comes from many different sources, among which we will mention parameters with uncertain values, uncertainty in the model as a representation of the underlying phenomenon, process, or system, and uncertainty in collecting/processing/measurements of data for model calibration. The task of quantifying and mitigating these uncertainties in mathematical models leads to the development of new statistical/stochastic methods, along with methods for efficient integration of data and simulation.

Further to supporting theories and increasing our predictive capabilities, mathematical and computational modeling can often suggest sharper natural experiments and more focused observations, providing in their turn a check to the model accuracy. Natural experiments and results of observations may produce large amounts of data sets that can intelligently be processed only with efficient mathematical data mining algorithms, powerful statistical and visualization tools [15]. The application of these algorithms and tools require a close collaboration between different disciplines. As a result, observations and experiments, theory and modelling reinforce each other, leading together to our better understanding of phenomena, processes, and systems we study, as well as to the necessity of even more close interactions between mathematical modelling, computational analyses and experimental approaches.

3   What This Book is About

The rest of the book consists of four main sections, containing eleven state-of-the-art chapters on applications of mathematical and computational modeling in natural and social sciences, engineering, and the arts. These chapters are based on selected invited contributions from leading specialists from all over the world. Inevitably, given the vast range of research areas within the field of mathematical and computational modeling, the book such as this can present only selective topics. At the same time, these selective topics open to the reader a broad spectrum of methods and tools important in these applications, and ranging from infectious disease dynamics and epidemic modeling to superconductivity and quantum mechanical challenges, from the models for voting systems to the modeling of musical rhythms. The book provides both theoretical advances in these areas of applications, as well as some representative examples of modern problems from these applications. Following this introductory section, each remaining section with its chapters stands alone as an in-depth research or a survey within a specific area of application of mathematical and computational modeling. We highlight the main features of each such chapter within four main remaining sections of this book.

- **Advanced Mathematical and Computational Models in Physics and Chemistry.** The section consists of three chapters.

  - This section is opened by a chapter written by I.M. Sigal who addresses the macroscopic theory of superconductivity. Superconducting vortex states provide a rich area of research. In the 1950-ies A. Abrikosov solved the Ginzburg–Landau (GL) equations in an applied magnetic field for certain values of GL parameter (later A. Abrikosov received a Nobel Prize for this work). This led to what

is now known as the famous vortex solution, characterized by the fact that the superconducting order parameter contains a periodic lattice of zeros. In its turn, this led to studies of a new mixed Abrikosov vortex phase between the Meissner state and the normal state. The area keeps generating new interesting results in both theory and application. For example, unconventional vortex pattern formations (e.g., vortex clustering) were recently discovered in multiband superconductors (e.g., [17] and references therein). Such phenomena, which are of both fundamental and practical significance, present a subject of many experimental and theoretical works. Recently, it was shown that at low temperatures the vortices form an ordered Abrikosov lattice both in low and high fields. The vortices demonstrate distinctive modulated structures at intermediate fields depending on the effective intervortex attraction. These and other discoveries generate an increasing interest to magmnetic vortices and Abrikosov lattices. Chapter by I.M. Sigal reminds us that the celebrated GL equations form an integral part, namely the Abelian-Higgs component, of the standard model of particle physics, having fundamental consequences for many areas of physics, including those beyond the original designation area of the model. Not only this Chapter reviews earlier works on key solutions of the GL model, but it presents some interesting recent results. Vortex lattices, their existence, stability and dynamics are discussed, demonstrating also that automorphic functions appear naturally in this context and play an important role.

– A prominent role in physics and chemistry is played by the Hartree-Fock method which is based on an approximation allowing to determine the wave function and the energy of a quantum many-body system in a stationary state. More precisely, the Hartree-Fock theoretical framework is based on the variational molecular orbital theory, allowing to solve Schrödinger's equation in such a way that each electron spatial distribution is described by a single, one-electron wavefunction, known as molecular orbital. While in the classical Hartree-Fock theory the motion of electrons is uncorrelated, correlated wavefunction methods remedy this drawback. The second chapter in this section is devoted to a multi-reference local correlation framework in quantum chemistry, focusing on numerical challenges in the Cholesky decomposition context. The starting point of the discussion, presented by D. K. Krisiloff, J. M. Dieterich, F. Libisch, and E. A. Carter, is based on the fact that local correlation methods developed for solving Schrödinger's equation for molecules have a reduced computational cost compared to their canonical counterparts. Hence, the authors point out that these methods can be used to model notably larger chemical systems compared to the canonical algorithms. The authors analyze in detail local algorithmic blocks of these methods.

– Variational methods are in the center of the last chapter of this section, written by M. Levy and A. Gonis. The basic premises here lie with the Rayleigh-Ritz variational principle which, in the context of quantum mechanical applications, reduces the problem of determining the ground-state energy of a Hamiltonian system consisting of N interacting electrons to the minimization of the energy functional. The authors then move to the main part of their results, closely connected to a fundamental element of quantum mechanics. In particular, they provide two alternative proofs of the generalization of the variational theorem for Hamiltonians of N-electron systems to wavefunctions of dimensions higher than N. They also discuss possible applications of their main result.

- **Mathematical and Statistical Models in Life Science Applications.** This section consists of two chapters.

  – The first chapter deals with mathematical modeling of infectious disease dynamics, control and treatment, focusing on a model for the spread of tuberculosis (TB). The latter is considered to be the second highest cause of infectious disease-induced mortality after HIV/AIDS. Written by J.

Arino and I. A. Soliman, this chapter provides a detailed account of a model that incorporates three strains, namely (a) drug sensitive, (b) emerging multi-drug resistant, (c) extensively drug-resistant. The authors provide an excellent introduction to the subject area, followed by the model analysis. In studying the dynamics of the model, they characterize parameter regions where backward bifurcation may occur. They demonstrate the global stability of the disease free equilibrium in regions with no backward bifurcation. In conclusion, the authors discuss possible options for their model improvement and how mathematical epidemiology contributes to our better understanding of disease transmission processes and their control.

– Epidemiological modeling requires the development and application of an integrated approach. The second chapter of this section focuses on these issues with emphasis on antibiotic resistance. The chapter is written by E. Y. Klein, J. Chelen, M. D. Makowsky, and P. E. Smaldino. They stress the importance of integrating human behaviour, social networks, and space into infectious disease modelling. The field of antibiotic resistance is a prime example where this is particularly critical. The authors point out that the annual economic cost to the US health care system of antibiotic-resistant infections is estimated to be \$21-\$34 billion, and given human health and economics reasons, they set a task of better understanding how resistant bacterial pathogens evolve and persist in human populations. They provide a selection of historical achievements and limitations in mathematical modeling of infectious diseases. This is followed by a discussion of the integrated approach, the authors advocate for, in addressing the multi-faceted problem of designing innovative public health strategies against bacterial pathogens. The interaction of epidemiological, evolutionary, and behavioral factors, along with cross-disciplinary collaboration in developing new models and strategies are becoming crucial for our success in this important field.

● **Mathematical Models and Analysis for Science and Engineering.** This section consists of four chapters.

– The first Chapter is devoted to mathematical models in climate modelling, with a major focus given to examples from climate atmosphere-ocean science (CAOS). However, it covers potentially a much larger area of applications in science and engineering. Indeed, as pointed out by the authors of this Chapter, D. Giannakis and A. J. Majda, large-scale datasets generated by dynamical systems arise in a vast range of disciplines in science and engineering, e.g. fluid dynamics, materials science, astrophysics, earth sciences, to name just a few. Therefore, the main emphasis of this Chapter is on data-driven methods for dynamical systems, aiming at quantifying predictibility and extracting spatio-temporal patterns. In the context of CAOS, we are dealing with a system of time-dependent coupled nonlinear Partial Differential Equations (PDEs). The dynamics of this system takes place in an infinite-dimensional phase space, where the corresponding equations of fluid flow and thermodynamics are defined. In this case, the observed data usually correspond to well-defined physical functions of that phase space, e.g. temperature, pressure, or circulation, measured over a set of spatial points. Data-driven methods appear to be critical in our better understanding of many important phenomena intrinsic to the dynamics of climate system, including El Nino Southern Oscillation in the ocean and the Madden-Julian Oscillation in the atmosphere. The authors provide a comprehensive review on data-driven methods and illustrate their techniques with applications, most of which are pertinent to CAOS. They conclude with a discussion of open problems and possible connections between the developed techniques.

– Inverse problems lie at the heart of many scientific and engineering inquiries. Broadly speaking, they provide a framework which is used to convert observed measurements (or desired effects) into

information about a physical object or system (or causes). This framework covers an extremely diverse range of applications, from imaging science, computer graphics and computer vision, to earth science, and to astrophysics. Many problems from life sciences, discussed in the previous section, can also be formulated as inverse. Some specific examples from science and engineering include the development of underwater detection devices, location of oil and mineral deposits, creation of astrophysical images from telescope data, finding cracks and interfaces within materials, shape optimization, etc. Regularization techniques are fundamental in solving inverse problems efficiently, and the Tikhonov regularization technique plays a particularly prominent role in this. In this Chapter, written by B. Hofmann, the author provides an overview of a number of new aspects and recent developments in Tikhonov's regularization for nonlinear inverse problems. The author formulates such problems as operator equations in Banach spaces. In order to construct stable and convergent approximate solutions to these problems, stabilizing penalty functionals are necessary. The author discusses in detail the interplay of convergence properties and approximate choices of the regularization parameters, as well as solution smoothness and the nonlinearity structure. In order to express and characterize the latter properties, a number of variational inequalities were presented. Examples on how to construct such inequalities were given, and their significance for obtaining convergence rates was also discussed.

– It is well known that many mathematical models, which play a fundamental role in science and engineering, can be formulated in the form of first order symmetric hyperbolic systems of differential equations, supplemented by constraints. Examples include Maxwell's equations, as well Einstein's field equations, to name just a few. If we consider the initial value (Cauchy) problem for either Maxwell's or Einstein's equations, it is known that the constraints will be preserved by their evolution. In other words, whenever the initial data satisfy the constraints, the solution will satisfy them too for all times. This is a starting point of the discussion in the Chapter written by N. Tarfulea. The author explains that for bounded computational domains, for example, artificial space cut offs may be needed for such evolution systems.The task then is to impose appropriate boundary conditions so that the numerical solution of the reduced (or cut off) system would approximate (in the best possible way) the original model defined on infinite space. The author provides a survey of known techniques for finding constraint preserving boundary conditions for some constrained first order symmetric hyperbolic systems (FOSH), followed by a number of new ideas for such constructions. Theory is exemplified by a constrained FOSH originating from a system of wave equations with constraints, as well as by more complex systems. In particular, Einstein's equations in the Einstein-Christoffel and Alekseenko-Arnold formulations are also analyzed with the proposed methodology.

– An overview of recent developments in methodologies for empirical organization of data is given in the Chapter written by R. R. Coifman, R. Talmon, M. Cavish, and A. Haddad. Through these methodologies, this Chapter provides a link between various applications of mathematics, ranging from natural sciences to engineering and to social sciences and the arts. Based on geometric and analytic ideas, the authors present a general mathematical framework for learning. These ideas are centered around building a network or a graph whose nodes are observations. In this framework, the authors propose maintain connections between observations by constantly reconfiguring them and calibrating in order to achieve learning characteristics for specific tasks. The developed methods are then related to ideas from Harmonic Analysis. The intrinsic connection between harmonic analysis and other disciplines is well known. Indeed, this area of mathematics is central to a wide range of applications, from signal and image processing to machine learning, quantum mechanics, to neuroscience and biomedical engineering. It enriches the rapidly growing field of data representation and analysis, and stimulate interdisciplinary research. The authors of this Chapter illustrate their ideas

on examples taken from both natural and social sciences. They show how such different things as text documents, psychological questionnaires, medical profiles, physically measured engineering data, or financial data, can be organize and map out in an automatic and purely data-driven manner.

- **Mathematical Methods in Social Sciences and Arts.** This section consists of two chapters.

  - This section is opened by Chapter written by S. J. Brams and D. M. Kilgour. It provides an important example of application of mathematical models in social and behavioral sciences. The range and diversity of such applications and developed models are growing continuously, from mathematical demography to models of contagion in finance, social dynamics and networks, arms races, social mobility, coalitions and consensus formation, quantification of power, experimental games, reduction of structural complexity, and decision theory. A notable example, presented in this Chapter deals with approval voting (AV). It is a voting system in which voters can vote for, or approve, as many candidates as they like. The authors proposed a new voting system for multiwinner election, called satisfaction approval voting (SAV). They considered the use of this system in different types of elections. For example, they considered a case where there are no political parties, as well as a number of other possible cases. Their system elects the set of candidates that maximizes the satisfaction of all voters, where a candidate's satisfaction score is the sum of the satisfactions that her/his election would give to all voters, while a voter's satisfaction is the fraction of her/his approved candidates who are elected. The authors demonstrated that SAV and AV may elect disjoint sets of candidates. In this context, an example of a recent election of the Game Theory Society was given. In conclusion, the authors explained why the most compelling application of their SAV is to party-list systems. This observation has important social implications, because SAV is likely to lead to more informed voting and more responsive government in parliamentary systems.

  - The concluding chapter of this section and the book provides an example of application of mathematical methods to arts, focusing on music, an art form whose medium is sound and silence. Ancient civilizations, including Egyptians, Chinese, Indian, Mesopotamians, and Greek, studied mathematics of sound. The expression of musical scales in terms of the ratios of small integers goes deep into the human history. Harmony arising out of numbers were sought in all natural phenomena by the Ancient Greeks, starting from Pythagoras. The word "harmonikos" was reserved in that time for those skilled in music. Nowadays, we use the word "harmonics" indicating waves with frequencies that are integer multiples of one another. The applications of mathematical methods from number theory, algebra, and geometry in music are well known, as well as the incorporation of Fibonacci numbers and the golden ratio in musical compositions. The concluding Chapter, written by G. T. Toussaint, is devoted to the field of evolutionary musicology where one concerns with characterizing what music is, determining its origin and cross-cultural universals. The author notes that a phylogeny of music may sometimes be correctly constructed from rhythmic features alone. Then, a phylogenetic analysis of a family of rhythms can be carried out based on dissimilarity matrix which is calculated from all pairs of rhythms in the family. How do we define musical rhythms? How do we analyze them? Asking these questions, the author provides a comprehensive account to what is known in this field, focusing on the mathematical analysis of musical rhythms. The working horse of the discussion is the well-known clave son rhythm popular in many cultures around the world. The main methodology developed for the analysis is based on geometric quantization. Different types of models are considered and compared, highlighting most important musicological properties.

4   Concluding Remarks

Mathematical and computational modeling, their methods and tools are rapidly becoming a major driving force in scientific discovery and innovation, providing us with increasingly more reliable predictive capabilities in many areas of human endeavor. In this section we have presented a brief historical account and an overview of new trends in this field, demonstrating universality of mathematical models. We highlighted a unique selection of topics, representing part of a vast spectrum of the interface between mathematics and its applications, that are discussed in detail in subsequent sections of the book. These topics cover mathematical and computational models from natural and social sciences, engineering, and the arts.

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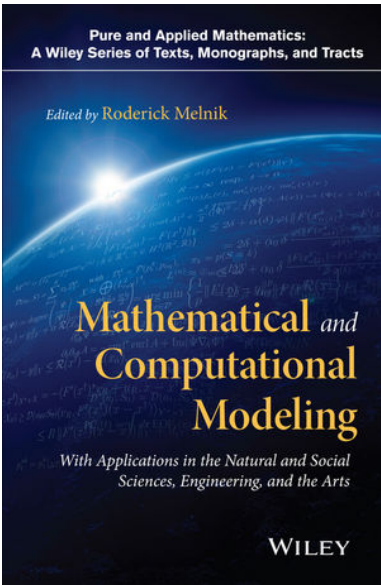
Mathematical and Computational Modeling: With Applications in Natural and Social Sciences, Engineering, and the Arts

Roderick Melnik (Editor)

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