Modern Challenges and Interdisciplinary Interactions via Mathematical, Statistical, and Computational Models

Roderick Melnik, Roman Makarov, and Jacques Belair

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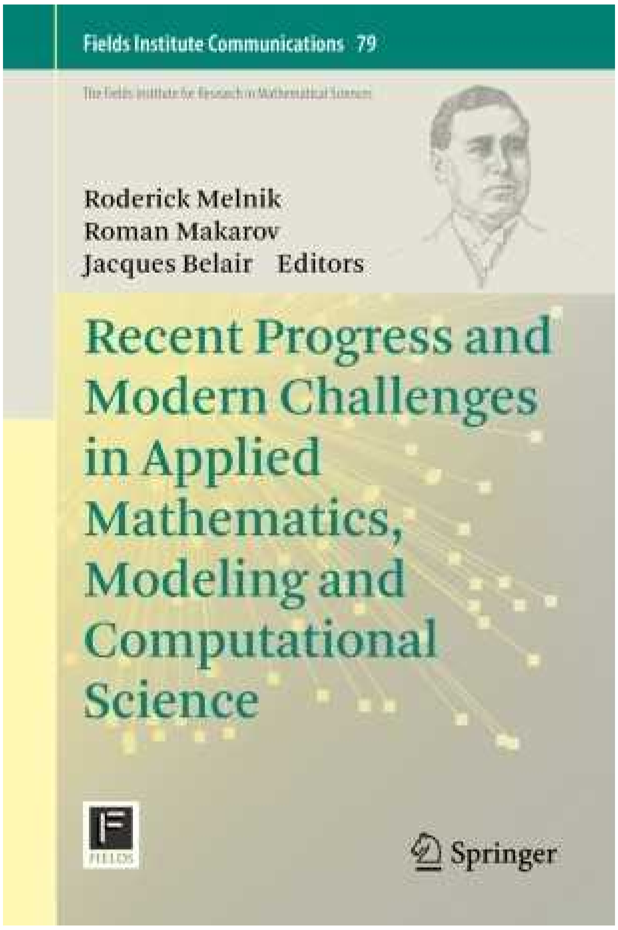

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Editors

Recent Progress and Modern Challenges in Applied Mathematics, Modeling and Computational Science

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Preface

The application of mathematics and statistics in the age of computational science and engineering has transformed our society and has revolutionized the world we live in. Being some of the oldest cultural achievements of mankind, nowadays these disciplines are intrinsic part of our daily life through our activities and technologies, ranging from our banking and investment systems to new sophisticated electronic devices, and to our civil infrastructure and environment.

These disciplines continuously grow at their frontiers though new areas of applications, new theories, and new tools provided by mathematical and statistical models. As a result, they continue representing the core of human knowledge critical for new discoveries and innovation, our well-being, and our economic prosperity.

There has been a long and rich interplay between mathematics and statistics on the one hand and other disciplines on the other, resulting in their fruitful enrichments. With ever-expanding interdisciplinary horizons of applied mathematics and statistics, we see new progress and modern challenges in their development. This book is about such progress and challenges in applied mathematics, modelling, and computational science.

Today, mathematical and statistical models are applied in natural and social sciences, industry and technology, medicine and finance. They are at the heart of a multitude of human activities, allowing connecting such activities in a modern world, where our communication gets better, faster, and cheaper also due to mathematics-based models. They substantially contribute to our better understanding of complex systems and networks whose components interact in a dynamic manner. Furthermore, mathematics-based computational technologies enable us detailed simulations of complex systems in the areas where the knowledge about such systems has been limited until very recently. Many such systems are functioned in a competitive, and often uncertain, environment. Therefore, the development of mathematical and statistical based methodologies of uncertainty quantification, as well as addressing other associated challenges, is essential.

Along with more traditional applications of mathematics and statistics in physics and engineering, we are witnessing now substantial contributions of these disciplines to new breakthroughs in biology and medicine, finance, and social sciences.

Equally important, mathematical and statistical models allow us to develop new important insight and better understanding of environmental and ecological sustainability in our dynamic and complex world.

This book provides details on recent progress and challenges in selected areas of applied mathematics, modelling, and computational science. It contains 14 chapters which open to the reader details on state-of-the-art achievements in these selected areas. The book provides a balance between fundamental theoretical and applied developments, emphasizing interdisciplinary nature of modern trends in these areas.

Written by 27 experts in their respective fields, the book is aimed at researchers in academia, practitioners, and graduate students. It can serve as a reference in the diverse selected areas of applied mathematics, modelling, and computational science. The book promotes interdisciplinary collaborations in addressing new challenges in these areas.

We are thankful to the referees of this volume for their invaluable help and suggestions. We are also very grateful to the Springer editorial team, and in particular to Dahlia Fisch, for their highly professional support.

Waterloo, ON, Canada — Roderick Melnik
Waterloo, ON, Canada — Roman Makarov
Montreal, QC, Canada — Jacques Belair

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CHAPTER 1

Modern Challenges and Interdisciplinary Interactions via Mathematical, Statistical, and Computational Models

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Abstract.

We live in an incredible age. Due to extraordinary advances in sciences and engineering, we better understand the world around us. At the same time, we witness profound changes in the technology, environment, societal organization, and economic well-being. We face new challenges never experienced by humans before. To efficiently address these challenges, the role of interdisciplinary interactions will continue to increase, as well as the role of mathematical, statistical, and computational models, providing a central link for such interactions.

1. The Role of Mathematical and Statistical Models

Since the dawn of human civilizations, technological innovations have been developing hand in hand with progress in mathematical and statistical sciences. Interactions and interdependence of mathematics, physics, engineering, and biology have been well elucidated in the literature with a number of excellent reviews and historical accounts (e.g., [12,13,19] and references therein). In the heart of these interactions and interdependence are mathematical and statistical models. Their role will continue to increase rapidly in both traditional (e.g., physics and engineering) and many emerging (e.g., health and life sciences) areas of their applications (e.g., [10,15,18] and references therein). Moreover, we are witnessing a dramatic increase in computing power and breathtaking advances in computational science and engineering which assist further in developing this trend.

Today, many other disciplines are catching up with this trend too. Indeed, mathematical and statistical models can be used to describe complex phenomena and systems such as stock markets, the internet traffic, logistics, supply, and demand of industrial networks, as well as climate change dynamics. Many complex systems that appear in nature, engineering applications, and society have components that interact in a remarkably dynamic manner in competitive, and often uncertain, environments. In order to understand them better, there is a need to develop new mathematical, including stochastic, models, as well as new methods for uncertainty quantification.

New challenges in of the modern world and our society require researchers working on many problems in economics and finance, social, environmental, and management sciences look for the development of quantitative models based on mathematical and statistical theories, methods, and tools.

As a result, new scientific, technological, and societal challenges we face in the 21st century can only be efficiently addressed in close collaboration with mathematicians and statisticians developing such quantitative models. At the same time, such challenges will stimulate the development of new concepts and theories in mathematical and statistical sciences, leading to many new breakthroughs in these two-way interactions between mathematics and statistics on the one hand and other disciplines on the other.

2. Application Areas and State-of-the-Art Developments

From a wide and increasing spectrum of applications of mathematical, statistical, and computational models, we selected some representative areas of these applications. Thus, the rest of the book consists of eight sections based on these areas. They contain state-of-the-art chapters, written by leading specialists from all over the world.

In selecting our areas for this book we intended to open to the reader a rich field of interdisciplinary interactions between many different disciplines with their unifying thread via mathematical and statistical models. The book provides details on theoretical advances in these selected areas of applications, as well as representative examples of modern problems from such applications. It also exposes the reader to open and emerging problems, and to challenges that lie ahead in addressing such problems.

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, statistical and computational modeling. Next, we highlight the main features of each such chapter within remaining sections of this book.

2.1. Large Deviation Theory and Random Perturbations of Dynamical Systems with Applications

Large deviation theory provides an important framework for modern statistical mechanics and stochastic system/process modelling. It allows us to describe the asymptotic behaviour of remote tails of sequences of probability distributions. Within this framework, many concepts of equilibrium statistical mechanics, such as entropy or free energy, can be considered as large deviation rate functions and can be generalized to the non-equilibrium case. Moreover, today this theory is considered to be one of the major tools for our better understanding of statistical information about complex dynamical systems, including the information on their most probable states, rare events, extremes, attractors, and typical fluctuations.

It is well known that long-time evolution of dynamical systems can be seriously affected by small random perturbations, leading to a lasting effect on their evolution. They can bring metastability, pronounced in transitions between otherwise stable equilibria [28], the phenomenon that is observed in a wide range of applications such as fluid dynamics, chemical reactions, population dynamics, and neuroscience. The mechanism of this phenomenon can also be explored with large deviation theory. A key element in the application of large deviation theory in this case is the path of maximum likelihood of such transitions. Moreover, the path itself can be computable through a numerical optimization problem as the minimizer of a certain objective function, known as action.

This section of the book, written by T. Grafke, T. Schafer, and E. Vanden-Eijnden, provides a review of theoretical foundation of large deviation theory that led to the rate function minimization problem. In particular, the authors are focusing on the geometric variant of this problem that is fundamental to the geometric minimum action method. They have proposed a new algorithm that simplifies this latter method. The authors demonstrate a considerable potential of their developed algorithm for a range of applied problems, including examples ranging from fluid dynamics and materials science to reaction kinetics and climate modelling.

2.2.Nonlinear waves, Hyperbolic Problems, and their Applications

For centuries the development of mathematical models and studies of waves have fascinated many researchers. Already Pythagoras analyzed waves through the relation of pitch and length of string in musical instruments. Today, the role of wave equations in the modern science and engineering is hard to overestimate. They are applied in classical and quantum mechanics, materials science and biology, medicine and finance, climate studies and social science. It is also an active area of theoretical research which includes the development of analytical and computational techniques and important connection to other areas of mathematics [23].

Originally presented in the context of physics applications, coherent states play an important role in nonlinear wave equations. In particular, such states are considered as quasi-classical states in quantum mechanical applications. Today the concept has been generalized to a number of other areas of mathematical physics and beyond (e.g., [5,27]).

The first chapter of this chapter, written by E. Kirr, starts from a general Hamiltonian formulation applicable to a large class of models related to wave propagation. Apart from the classical wave equation, this includes mathematical models based on Schrödinger's, Hartree's, Dirac's, Klein-Gordon's, Kortweg-de-Vries' equations. The author demonstrates that while large coherent structures can be found via variational methods (e.g., as minimizers of the energy, subject to a fixed value on the second conserved property), this is not the case for the problems where all coherent states are required. To address this challenge the author proposes to apply the analytical global bifurcation theory for finding all coherent states, as well as for analyzing orbital stability of such states. Within this framework, the author provides details on how to study asymptotic stability of coherent states, as well as on long-time behaviour of nearby solutions, and identifies some open problems in this field. For example, despite the recent progress in asymptotic stability near an orbitally stable coherent state, in the general case we still do not know how to determine the full dynamic picture near a bifurcation point.

Hyperbolic equations are in the heart of discussion in the second chapter of this section, written by R. Abgrall, who deals with both linear and non-linear problems. The main focus is on the development of parameter-free methods for scalar hyperbolic equations that satisfy a local maximum principle. The author presents a systematic methodology for constructing higher order finite element type methods satisfying this principle. The results are not limited to the problems with regular solutions only. A detailed analysis of conditions that guarantee the convergence of the developed numerical scheme to weak solutions under stability assumptions has been provided. Furthermore, the author has provided the conditions that guarantee an arbitrary order of accuracy of the developed scheme. Generalizations of the proposed methodology have also been discussed in the context to its extensions to systems, including Euler's equations and the Navier-Stokes model. Among the remaining challenges the author highlights the importance of a better design of the filtering parameter.

2.3.Group-Theoretical Approaches to Conservation Laws and Their Applications

Numerical integrators, where we preserve exactly one or more properties of the original differential-equation-based mathematical model, has been a subject of interest for a long time, with a number of excellent reviews, books, and journal special issues published (e.g., [3,11,26] and references therein). Given that geometric properties of the exact flow of the underlying differential equation are typically preserved in such cases, we call the associated integrators structure-preserving or geometric numerical integrators. While this type of methodologies has largely been developed for ordinary differential equations, there are important results in the development of these ideas to partial differential equations too (e.g., [4,20,21]). These methodologies, applied to both deterministic and stochastic systems, have been developed in parallel, and often independently, from energy-conserving methods (e.g., [1,16,25] and references therein). Such methods are typically derived for the variational formulation of the problem and can be applied to both Lagrangian and Hamiltonian dynamics.

The underlying success of variational integrators, leading to their numerous applications, lies with their group-theoretical foundation and Lie group analysis which has been well elucidated in the literature (e.g., [14] and references therein). For example, applied to Lagrangian dynamical systems, they preserve a discrete multisymplectic form, as well as momenta associated to symmetries of the Lagrangian via Noether's theorem. As it was pointed out in [17], a prerequisite of obtaining variational integrators is the existence of a variational formulation for the considered dynamical system. Not all systems in applications are of this type. Examples of non-variational mathematical models based on partial differential equations can be found in such areas as plasma physics, fluid dynamics, as well as in magnetohydrodynamics, to name just a few. As a result, there is an increasing interest to a generalization of Noether's theorem to handle such cases too. Recent attempts in this direction include a discrete version of the Noether theorem for formal Lagrangians that yields the discrete momenta preserved by the resulting numerical schemes [17]. The method, based on the embedding of a dynamical system into a Lagrangian system by doubling the number of variables, has been applied to Vlasov-Poisson and magnetohydrodynamic systems, as well as to non-canonical Hamiltonian systems.

This section is a comprehensive review, written by S. Anco, discussing other generalizations of Noether's theorem to non-variational mathematical models based on partial differential equations. One of the major concepts is that related to multipliers, the expressions whose summed products with a PDE-based system yields a local divergence identity. The latter is associated with a continuity equation involving a conserved density and a spatial flux for solutions of the underlying PDE. The author demonstrates that when the underlying model is non-variational, such multipliers are an adjoint counterpart to infinitesimal symmetries. Moreover, the local divergence identity, that relates a multiplier to a conserved integral, appears to be an adjoint generalization of the variational identity that underlies Noether's theorem. A procedure for computation of multiplies has been described in detail.

2.4. Materials Science, Engineering, and New Technologies

Computer-aided innovation of new materials is an important area of research in materials science and engineering. The development of computationally efficient approaches and modelling in this field has been a subject of immense research interest ever since our advances in computational power [7,22]. This includes innovative superhard materials, as well as smart materials such as superelastic and shape memory alloys [6]. A large class of such materials are binary alloys. For binary alloys, the most accurate energy calculations are typically done via the density functional theory, and as any *ab initio* calculations this methodology is computationally very expensive.

The first chapter in this section, written by J. Kristensen, I. Bilionis, and N. Zabaras, discusses viable alternatives to the above methodology. They argue that in this area of applications it is important to devise new schemes for the automatic and maximally informative selection of simulations. They provide a detailed description of their developed information acquisition policy for learning the ground state of binary alloys. Starting from the surrogate modelling technique and presenting the energy computation scheme, the authors describe their theoretical approach, based on a Bayesian interpretation of the cluster expended energy. Their developed framework for selecting structures has been extended to account for the effect of alloy structure costs. By comparisons with other structure acquisition algorithms, it has been concluded that optimal information acquisition policies should balance the maximization of the expected improvement of the ground state line and the minimization of the size of the simulated structure. The developed approach has been validated for a number of important binary alloys, including NiAl and TiAl. Once a probabilistic surrogate of the relevant thermodynamic potential is constructed, the proposed policies can be directly applied to the discovery of generic phase diagrams.

The second chapter of this section, written by P. Fischer, M. Schmitt, and A. Tomboulides, presents a comprehensive overview of spectral element methods for an important class of fluid dynamics problems. Their focus is on incompressible and low-Mach-number flows in domains with moving boundaries. From applications of these mathematical models, it is well known that moving boundaries introduce new sources of nonlinearity and stiffness [9]. For example, in fluid-structure interaction problems, one of the reasons for that lies with disparate time scales between the fluid and solid responses. A similar situation holds for other coupled problems. The authors pay special attention to recent developments addressing these moving-domain challenges, while keeping the computational efficiency required for turbulent flow simulations. One of the important features in their discussion is an arbitrary Lagrangian-Eulerian formulation for low-Mach-number flows that includes an evolution equation for the background thermodynamic pressure. A rich selection of numerical examples has also been provided to illustrate main theoretical results.

The concluding chapter of this section, written by C. Budd, offers an exciting journey into mathematical foundations of new technologies. The author reviews eight such technologies, identified by the UK government as those that would act as a focus for future scientific research and funding. They are

a) Big Data

b) Satellites and space
c) Robotics and autonomous systems
d) Synthetic biology
e) Regenerative medicine
f) Agricultural science
g) Advanced materials
h) Energy and its storage.

Based on a historical account and recent progress, the author demonstrates that mathematics lies at the heart of all of them, linking them all together. A number of challenges, both mathematical and interdisciplinary, have been determined and discussed in the context of future development of these technologies.

2.5.Finance and Systemic Risk

This section contains three chapters. It is opened by a chapter written by Q. Feng and C. Oosterlee addressing the problem of credit valuation adjustment. The authors pointed out that this quantity is required in the Third Basel Accord - a global framework on bank capital adequacy, stress testing, and market liquidity risk - that came around in the wake of the credit crisis. In calculating credit valuation adjustment, exposure is a key element. This characteristic is defined as the potential future loss on a financial contract due to a default event. The chapter describes a backward-dynamics-based general framework for calculating exposure profiles for different options, enabling us to analyze the sensitivity of the model to such options. The authors focus on two models, the Heston and Heston-Hull-White asset dynamic models, which they consider under European, Bermudan, and barrier options. In particular, for these models and options they describe their generalization of the Stochastic Grid Bundling Method for the computation of exposure profiles and sensitivity for asset dynamics. This generalization provides a flexible valuation framework for credit valuation adjustment. Details are given for the most important features of the developed methodology, including the choice of the basis functions for the local regression, the convergence of the direct and path estimators with respect to an increased number of bundles, and the associated accuracy. A series of numerical tests presented in this chapter demonstrated these features in practice, also showing that the computational efficiency of the developed methodology is connected to the number of bundles used in the

Stochastic Grid Bundling Method. A drastic reduction in computational time is achieved with a parallel implementation of the developed algorithm.

The next chapter is this section, written by T. Bielecki, J. Jakubowski,a nd M. Nieweglowski, is devoted to recent progress in the emerging theory and practice of structured dependence between stochastic processes. It is argued that our success in this field will be dependent on our ability to construct different types of Markov copulae [2]. The authors of this chapter present a new result on independence copula for conditional Markov chains. A copula can be used to describe the dependence between random variables. It is a multivariate probability distribution for which the marginal probability distribution of each variable is uniform. The authors of this chapter describe how to construct the conditionally independent Markov copula (or the conditionally independent multivariate Markov coupling) for a family of conditional Markov chains. While the reported result is important in finance applications, e.g. in modelling credit rating migrations, there is a range of its possible applications in other areas. One of the challenges in this field, identified by the authors, is to effectively construct weak Markov copulae and weak conditional Markov chains.

This section is concluded by the chapter devoted to financial systemic risk models. Written by T. Hurd, its main result is in providing essential foundations needed to prove rigorous percolation bounds and cascade mapping in assortative networks. The main premises of the author's approach are based on the fact that the network of interbank counterparty relationships can be described as a directed random graph. When cascade models of financial systemic risk are used, the structure of this graph (or the skeleton of a financial network) can be thought as a medium through which financial contagion is propagated. The author focuses on a particular general class of random graphs – the assortative configuration model. A new approximate Monte Carlo simulation algorithm for assortative configuration graphs has been described in detail, and challenges for efficient simulations of such graphs have been highlighted.

2.6.Life and Environmental Sciences

Many problems in biology and life sciences require consideration of environmental effects. One class of such problems is related to the analysis of coexistence of interacting populations in uncertain environment.

This section, written by S. Schreiber, focuses on this class of problems accounting for random fluctuations due to both environmental and demographic stochasticities which are experienced by all populations. It is argued that demographic stochasticity can be represented by Markovian models with a countable number of states where quasi-stationary distributions of these models characterize metastable patterns of the system behaviour connected to long-term transients. At the same time, the effects of environmental stochasticity on population dynamics can be modelled with stochastic difference equations. The author explains that for these models, stochastic persistence would correspond to empirical measures placing arbitrarily little weight on arbitrarily low population densities. Sufficient and necessary conditions for such persistence are based on a weighted combination of Lyapunov exponents. The theory has been developed for both single-species and multi-species models.

The author has provided the reader with a range of interesting examples to support the developed theory. This includes the quantification of climatic variability effects on the dynamics of Bay checkerspot butterflies, the persistence of coupled sink populations, coexistence of competitors through the storage effect, and stochastic rock-paper-scissor communities. The chapter contains a comprehensive list of open problems and challenges in this field.

2.7. Number Theory and Algebraic Geometry in Cryptography and Other Applications

The topic of elliptic curves has an important place in mathematics and its applications. In the domain of applications this topic came to its new prominence in the late 70ies of the 20th century when public key cryptography and cryptosystems become important for private and secure electronic communication [8]. In 1993 it became also known that elliptic curves were used in Andrew Wiles' proof of Fermat's Last Theorem. With the astounding growth of the Internet and new security challenges of the 21st century, there is all evidence to expect increasing importance of elliptic curves in a number of application areas. Nowadays, the topic represents a combination of important challenges in practical/algorithmic issues and the underlying mathematical beauty with a range of open problems.

This section covers both computational/algorithmic and theoretical aspects of elliptic curves. Written by M. Bennett and A. Rechnitzer, the section provides a good introduction to ubiquitous nature of these structures in mathematical sciences, particularly in number theory and algebraic geometry. From a practical viewpoint, the authors focus on the problem of generating/tabulating elliptic curves with desired properties. Along with a comprehensive overview of state-of-the-art in the area, they provide details of an algorithm for computing models for all elliptic curves with integer coefficients and given conductor. The latter quantity has been studied since A. Ogg and A. Weil in the late 60ies of the previous century, and is often considered to be an integral ideal analogous to the Artin conductor of a Galois representation. In the context of the current section, the authors define it as an invariant that provides information about how a given elliptic curve behaves over finite fields. Based on extensive comparisons to existing data, they demonstrate that although their approach is based on classical ideas, it leads to a very efficient computational algorithm. Furthermore, given multiple examples and data provided in this section, the authors challenge the reader with new problems in this exciting area.

2.8.Sustainability and Cooperation

In many applications we have to deal with dynamic interactions of several entities, agents, or players, in such a way that we can achieve a long-term cooperation, stability, and sustainability. Many problems in economics, social, engineering, and management sciences are of this type. Additional examples include the interaction between economic and ecological dynamic systems or other systems where cooperation and negotiation on the amount and the allocation of investment could lead to more sustainable use of natural resources [24]. In many such cases, the dynamic coalition-formation process can be modelled via a self-organized transition from unilateral action (Nash equilibria) to multilateral cooperation (Pareto optima).

When we have only a few agents/players with interdependent playoffs, cooperating/competing repeatedly over time for resources under uncertainty (e.g., in demand), the general framework of dynamic games played over event trees is often most suitable way to formalize such problems mathematically.

In this section, written by G. Zaccour, all principle components of the theory of dynamic games played over event trees have been reviewed. Starting from a review of the literature pertinent to the sustainability of cooperation in dynamic games, the author moves to the details of the approach to achieve a node-consistent outcome in dynamic games played over event trees. This approach is illustrated by the node-consistent Shapley value, as well as by the node-consistent core. In a methodologically consistent manner, the author has demonstrated how sustainable cooperative solutions can be constructed. The chapter has also highlighted several open problems. For example, can cooperation still be sustained if the cores in some of subgames are empty? Another interesting problem is the analysis of node consistency for dynamic games played over event trees in the case when the end of the horizon is random.

3. Conclusions

In this section we highlighted a selection of areas, representing part of a broad spectrum of the interdisciplinary interface where mathematical, statistical, and computational models play a central role. Such models provide an indispensable tool for scientific discoveries and innovation in the areas ranging from physics and biology to economics and finance, from security and defense to sustainability studies.

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