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In: Fields Institute Communications, Vol. 66, pp. 1- 11, Springer, 2013.

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Print ISBN978-1-4614-5388-8 || Online ISBN978-1-4614-5389-5

Series Print ISSN1069-5265 || Series Online ISSN2194-1564

DOI: https://doi.org/10.1007/978-1-4614-5389-5

Interconnected Challenges and New Perspectives in Applied Mathematical and Computational Sciences

Roderick V. N. Melnik and Ilias S. Kotsireas

Abstract More and more disciplines increasingly rely in their progress on the development of mathematical models, methods, and algorithms. Mathematical modeling and computational science are seen as a driving force in scientific discovery and innovative, mathematics-based technologies. They can facilitate new advances in systems-science-based approaches in applications and serve as a decisive factor in sustainable socio-economic development of the society. The chapter provides an overview of these new trends.

1 Mathematical Models and Algorithms

The methods and ideas of mathematics are taking on new and new spheres of influence. This process, started well before the famous quote by Galileo Galilei that "the Book of Nature is written in the language of mathematics", can be traced back to the thoughts of Pythagoras' school, while the origin of its path is hidden at the dawn of human civilization. Today, all existing advanced information technologies are essentially *mathematics-based technologies*, including mobile communication and internet. Mathematical models and mathematics-based quantitative analyses have penetrated to and are becoming increasingly important in the areas that were only recently labeled as non-traditional for conventional mathematics, ranging from life science and medicine, to business and economics, and to social, political and forensic sciences, to name just a few. What made this process developing at a much faster pace than ever before, in the last 70 years or so, is the ready availability of computer

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R. Melnik, I. Kotsireas (eds.), *Advances in Applied Mathematics, Modeling, and Computational Science*, Fields Institute Communications 66,
DOI 10.1007/978-1-4614-5389-5_1, © Springer Science+Business Media New York 2013

power. This has led to a situation where many problems in sciences and engineering that could not be solved before found their way to be analyzed and explored computationally. Mathematics with its foundations in applications and computational science with its mathematics-based numerical *algorithms* become two wings of the same bird. What connects them together is the body of human knowledge which we call *mathematical modeling*. Under mathematical models we understand connections, patterns, or abstract constructs that characterize a phenomenon, a process, or a system such that they can be expressed in some mathematical form via equations, inequalities, formulae, sets of rules, etc. The original stimuli for the development of simplest mathematical models were agricultural needs of humans, subsequent development of geometric knowledge, arithmetics (as a precursor of number theory), and their applications. Probably, one of the most famous examples of such applications in the Ancient Times were the Egyptian Pyramids (with the earliest known, the Pyramid of Djoser, constructed 2630 BCE–2611 BCE). As pointed out by H. Poincare, "the true method of forecasting the future of mathematics lies in the study of its history and its present state" [1]. Many early examples of applications of mathematical knowledge demonstrate that such applications were closely interwoven with the development of mathematical algorithms, providing key stimuli for their applications. As abstract areas of mathematics are also based on models, mathematical algorithms have been fundamental in their development too. Unquestionably, algorithms are also central in computational mathematics, science, and engineering. The word "algorithm" stems from the name of Al-Khwarizmi (c. 780–c. 850), born in Khwarizm.[1] Translations of the works of this great scholar brought the decimal positional number system to the Western world, and the word "algorithm" was meant to indicate a technique with numerals. In the Ancient World, the development of algorithms was an important pillar of mathematical applications and was initially stimulated by geometrical considerations. Babylonian and Indian mathematicians already knew algorithms for approximating the area of a given circle. In the Ancient Greece, Antiphon the Sophist and Bryson of Heraclea in the 5th century BC were probably the first who developed an algorithm for calculating π by inscribing and then circumscribing a polygon around a circle, and calculating the polygons' areas. This methodology, known as the method of exhaustion, was a precursor to the integral calculus, and both Eudoxus of Cnidus and later Archimedes of Syracuse greatly contributed to its further development and applications. The development of number theory has also been a natural, rich source of algorithms. Early examples include Euclid's algorithm to determine the greatest common divisor of two integers, presented in his book the Elements. Later, the development of algorithms for finding solutions to mathematical models based on linear and non-linear equations, optimization and control problems has been dotted with the names of many outstanding scientists and mathematicians, including R. Descartes, I. Newton, L. Euler, C.F. Gauss, L. Kantorovich, G.B. Dantzig, J. von Neumann, L. Pontryagin, R. Bellman, and many others. While algorithms have always been central in the develop-

[1] Currently Khiva, Uzbekistan; geographically, Khwarizm or Chorasmia is a large oasis region on the Amu Darya river delta in western Central Asia.

ment of mathematical sciences, their importance has been substantially magnified with the advent of computers.

The speed of carrying out arithmetic and logical operations has increased drastically and continues to grow, leading to the ever increasing productivity in information processing and intellectual performance, not available to humans before. As a double-edge sword, this new power has to be used wisely and with caution. At the same time, it allows us to face new challenges in science, technology, and society. The process has led to an unprecedented boost in the development of new mathematical algorithms for the needs of computational science which has transformed the entire landscape of human activities, including scientific research, engineering design, production technologies, and education [2]. Through mathematical modeling, mathematics has become one of the major beneficiaries of this process, expanding its methods and tools to new areas. With the help of computational science, mathematical models now provide a stronger and more visible link between mathematics and the outside world, simultaneously strengthening links between different areas within mathematics itself.

2 Mathematical Modeling and Computational Experiments

The first step in mathematical modeling has always been to construct/derive a mathematical model. When studying phenomena, processes or systems in sciences and engineering or other areas of human endeavor, many mathematical models that are being constructed can be linked to the observable reality. In such cases, mathematical modeling can often complement natural experiments. The quality of mathematical models in such cases depends on the agreement between the results of mathematical modeling and natural experiments (experimental measurements). Therefore, the process of mathematical modeling is often a driving source for the development of new, better models, as well as for the development of hierarchies of mathematical models of different complexity (e.g., progressively more complex coupled models). This process helps determine the range of applicability of models and their possible simplifications. 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. Notwithstanding that models for the same system can involve a range of mathematical structures and can be formalized with various mathematical tools (equation-based models, graphs, logical and game theoretic models, etc.).

Traditionally, the analysis of mathematical models has been based on a simplification of the model and some a priori assumptions made in such a way that something can be said analytically. Frequently, however, such simplifications lead to unrealistic assumptions and, as a result, to a large deviation from the reality of the phenomenon, process or system that is being described by the original model. The modern development of science and engineering convincingly demonstrates that the class of the models amenable to such simplifications, while keeping assumptions realistic, is strikingly smaller compared to the general class of mathematical models that are at the forefront of modern applied mathematics, science, and engineering. As a rule, the problems in the latter class have to be treated numerically. Numerical methods for solving such problems require, in their turn, the development of efficient algorithms which are presented by sequences of mathematical/computational operations that would lead to a solution of the problem, often in the limit. Once such algorithms are implemented (programmed) computationally, we can run the model multiple times under varying conditions, helping us to answer outstanding questions quicker, more efficient, and providing us an option to improve the model when necessary. The triad "model-algorithm-implementation" is at the heart of mathematical modeling that leads to our ability to carry out *computational experiments* which become a pervasive and powerful theoretical tool in many areas of mathematical applications. Such areas embrace, for example, nonlinear phenomena in sciences and engineering, various spatio-temporal interactions, as well as complex systems studies, including the systems whose dynamics is only partially observable and systems with incomplete information.

While in the past, scientists, mathematicians, and engineers could use only simplified mathematical models to make them amenable to analytical treatments, the situation has now fundamentally changed. Indeed,

- we can now carry out computational experiments with more refined models, to solve them with more efficient methods, and to obtain more accurate results, unachievable with analytical techniques;
- we can carry out computational experiments in cases when natural experiments are impossible or difficult;
- with appropriate validation and verification procedures, we can provide reliable information more quickly and with less expense compared to natural experiments.

Computational experiments have become an intrinsic part of modern science and engineering and one of the essential tools in scientific discovery. Such experiments, sometimes referred to as "in silico", cover a wide spectrum of new computer-assisted disciplines such as computational physics, computational chemistry, computational materials science, computational biology, computational engineering, etc. In all these disciplines, we replace a traditional mathematical model by its computer equivalent, a computational model. Via computational experiments and theoretical analysis, we can assess the limits of applicability of mathematical models which can help set up natural experiments (sometimes referred to as "in vivo") and predict their results. This a two-way interaction. Indeed, most natural experiments are supported mathematically (via optimization of experiments, inverse problems, problems of identification, etc.). Not only can computational experiments be applied to traditionally applied areas of mathematical sciences mentioned above, but they can also be applied to their theoretical areas, and computational number theory, e.g., provides many beautiful examples. Even if an analytical solution to the original mathematical model is not known, based on a mathematical algorithm, a computer simulation can find an approximate solution. Computational experiments have promoted understanding in the society that new technologies developed with computational science and engineering tools are undoubtedly mathematics-based technologies.

An important feature of the current situation lies also in the fact that mathematical modeling becomes increasingly multidisciplinary. Computational science and engineering extend the applications of mathematics to new areas, reaffirming the versatility and ubiquitous nature of mathematical modeling. This provides new challenging problems in applied mathematics. At the same time, the development and implementation of new algorithms in these areas is closely connected with the development of information technology. Indeed, it is hard to overestimate the importance of the analysis of algorithms for emerging computer architecture. These two-way interactions, between information technology on the one hand and mathematical modeling and computational science on the other, continue to have a substantial impact on the analysis and *predictive capabilities* of mathematical models.

3 What Is Next

Computational experiments and the development of new methods and algorithms to support them help reveal some interconnected challenges in applied mathematical and computational sciences. Many systems that we encounter in nature, as well as man-made systems, are intrinsically inter-connected (coupled) with their parts interacting in non-trivial dynamic manner. Such systems require innovative mathematical and computational approaches, and their analysis demands fostering cross-fertilization between different disciplines and mathematics, as well as between different areas within mathematics. The areas where such systems frequently appear include, but not limited to:

- life sciences,
- earth, climate, environmental, and sustainability sciences,
- high energy and nuclear physics, fusion and energy problems,
- materials science and chemistry,
- cosmology, astrophysics, and celestial mechanics,
- aerospace sciences and new technologies,
- and others.

Facing many problems in these areas would require the development of new efficient algorithms, higher-order methods, systems-science-based approaches, and building multidisciplinary capabilities. New advances in mathematical modeling of intrinsically interconnected (coupled) systems will call upon an integration of a variety of methods and tools across multiple disciplines, including different areas of mathematics. Indeed, some such systems, especially those that are inherently stochastic and those with incomplete or partially observable dynamic behaviors, would require improved predictive capabilities of mathematical models describing them. The models in such cases should be able to predict the probability of an outcome in the best possible way. The success of predictive mathematical modeling is dependent also on further advances in information sciences, and the development of statistical and probabilistic methods, methods for uncertainty quantification, and machine learning techniques. Furthermore, since coupled systems are often interacting on a range of spatio-temporal scales, the development of predictive multiscale models and multiscale algorithms (in particular, for filtering and data assimilation and various types of parametrization) is becoming an important new avenue of research.

Probabilistic and applied statistics approaches will also become increasingly important in the design, analysis, and optimization of computational experiments. This is due to three main sources of uncertainty caused by (a) parameters with uncertain values, (b) uncertainty in the model as a representation of the underlying phenomenon, process, or system, and (c) uncertainty in collecting/processing/measurements of data for model calibration. In quantifying and mitigating these uncertainties in mathematical models, new developments in novel statistical-stochastic methods and methods for efficient integration of data and simulation are expected.

With an unprecedented growth of the range of application areas where mathematical modeling and computational science play an increasingly important role, demands for professions with adequate mathematical skills should increase. This raises a number of challenges in education of such future professionals at the university level, a topic which lies beyond the scope of this introductory chapter.

4 What This Book Is About

The rest of the book consists of eight state-of-the-art chapters on important recent advances in applied mathematics, modeling and computational science. These chapters are based on selected invited contributions from leading specialists from North America, Australia, and Europe.

The vast range of research areas within these three interconnected fields has led us to a selection of topics covered in this book. Hence, the chapters that follow provide a selective, but at the same time broad spectrum of methods and tools that are at the forefront of modern developments in applied mathematics, mathematical modeling and computational science. Each chapter has both theoretical and applied parts, making the book a comprehensive combination of mathematical theories, model derivations, and development of efficient numerical procedures applicable to a wide range of applications. The book contains also a selection of 12 computer codes, written in MATLAB in a simple and transparent way to allow the reader immediate access to the idea, as well as a variety of state-of-the-art numerical algorithms with applications in fields ranging from population dynamics and medicine to cryptography and fire propagation.

- *Dynamic blocking problems and their applications.* The theory of dynamic blocking problems has a number of various applications such as the propagation of a wild fire in a forest, various traffic problems, the spatial spreading of a contaminating agent, etc. A comprehensive survey of this theory is given by A. Bressan (Penn State University, USA). Mathematical models of dynamic blocking problems can often be cast in the form of differential inclusions describing the growth of sets in the plane. In order to restrain the expansion of such sets, it is usually assumed that barriers can be constructed. From both theoretical and practical points of view, it is important to be able to understand whether the growth of these sets can be blocked. Therefore, the author reviews the results known up to date on the existence and non-existence of blocking strategies. Another important issue addressed in this chapter is how to find the optimal location of the barriers, minimizing a cost criterion. The author provides all details on both necessary and sufficient conditions for optimality. He goes on to the description of a numerical algorithm for the computation of optimal barriers. The chapter is concluded with a survey of open problems in this new challenging area of research.

- *High order accurate numerical boundary conditions for solving hyperbolic equations.* The challenges of boundary treatment in mathematical models based on partial differential equations are well known in computational science and engineering. They are intrinsic to various numerical techniques applied for solving associated problems, including finite difference schemes and finite element type methods. A review and discussions on new developments in meeting these challenges are given in the current chapter by S. Tan and C.-W. Shu (Brown University, USA). They focus on the Inverse Lax-Wendroff (ILW) procedure and consider high order accurate finite difference methods for solving hyperbolic conservation laws involving complex static and moving geometries. Their methodology is applied on Cartesian grids, while the physical domain can be arbitrarily shaped. Some of the challenges that need to be address in this case include typically wide stencils for high order schemes and the fact that the grid lines may not necessarily coincide with the physical boundary. The authors give a very thorough description of their main methodology based on the ILW procedure for inflow boundary conditions and on a robust and high order accurate extrapolation for outflow boundary conditions. They provide details of the stability of the method, followed by a series of examples that include also problems involving interactions between shock waves and rigid boundaries.
- *Number theoretic and cryptographic issues of elliptic curves over finite fields.* Modern number theory has a rich history that can be traced back to the dawn of human civilization. The interest to elliptic curves is of more recent origin and one of the main reasons for the great interest to them for more than a century lies with the fact that they have a naturally associated with them group structure. A self-contained survey demonstrating strong links between many problems on elliptic curves over finite fields and a myriad of problems in analytic, algebraic, and computational number theory is given by I.E. Shparlinski (Macquarie University, Australia). The range of such problems has expanded further after the invention of elliptic curve cryptography, opening up many new research directions and applications. The author demonstrates that number theory remains central to both, a classical theory of elliptic curves and application driven research in these areas. After giving a detailed account of the structure of elliptic curves over finite fields, cryptographic applications of such curves are considered. The topics include, but not limited to, pairing friendly curves and pseudorandom number generators. The survey can serve as a reference for theoreticians to this new important direction,

as well as a source of new problems. It can be useful to the cryptographers and other practitioners working in applications of the modern number theory. The self-contained nature of the survey makes it also accessible to graduate students and those who are interested in learning about state-of-the-art developments in these areas.

- *Random matrix theory and its innovative applications.* Random matrices (matrix-valued random variables) are found an increasing number of applications in science and engineering. This process, starting at the beginning of the 20th century, has led to what we now know as Random Matrix Theory (RMT). Its many applications are often surprising and innovative. In number theory (see our previous chapter), for example, the distribution of zeros of the Riemann zeta function can be modelled by the distribution of eigenvalues of certain random matrices. Many novel examples of RMT applications are given in this chapter by A. Edelman (Massachusetts Institute of Technology, USA) and Y. Wang (Tufts University, USA). Such examples are ranging from health sciences to many engineering problems where the limiting densities are often needed to indicate the cutoff between "noise" and "signal". The chapter explains the theory behind these examples and associated applications. The reader can find here the Hermite and Laguerre ensembles, the description of four famous laws used in RMT as they govern the limiting eigenvalue distributions of random matrices. The details of matrix reductions and an overview of how these reductions can be used for efficient computation are also given. The chapter contains 12 codes, written in MATLAB, so that the readers can immediately embark on some of the RMT ideas in their specific areas of applications.
- *Energy stable weighted essentially non-oscillatory finite-difference schemes and their applications.* Complex scientific and engineering problems exhibiting discontinuities are ubiquitous in applications. For high fidelity simulations of such problems high-order weighted essentially non-oscillatory (WENO) schemes are often methods of choice. Near domain boundaries, however, these methods face serious challenges. Boundary closures of high order have recently been developed to overcome existing problems, as these closures, along with near-wall biasing mechanics, complement the periodic domain energy stable WENO methods (ESWENO). The chapter by M.H. Carpenter, T.C. Fisher (both NASA Langley Research Center, USA), and N.K. Yamaleev (North Carolina A&T University, USA) provides a summary of the recent developments in this field. It is demonstrated that a novel set of nonuniform flux interpolation points is necessary near the boundaries in order to simultaneously achieve accuracy, the summation-by-part convention, and WENO stencil biasing mechanics. One of the motivations for this work has been provided by simulations of sound that is generated by a shock-vortex interaction. Practical examples have been given to complement the theoretical part and to test the developed methodology. These include unsteady propagation of a two-dimensional Euler vortex and unsteady convection-diffusion-reaction of a supersonic hydrogen-air mixing layer, simulated by solving the two-dimensional Navier-Stokes equations. Detailed instructions on and numerical algorithms for the implementation of the new ESWENO schemes have also been provided.

- *Multiscale methods coupling network and continuum models in porous media.* Modeling transport in porous media applications is know to be a difficult task. This is especially true, for example, for two-phase flow simulations in porous media where nonlinearity and heterogeneity of small scale processes dictate the large scale flow behavior. This problem is addressed in the present chapter by J. Chu, B. Engquist, M. Prodanovic, and R. Tsai (all at the University of Texas at Austin, USA). They present a new numerical multiscale methodology for coupling a conservation law for mass at the continuum scale with a discrete network model that describes the pore scale flow in the porous medium. The developed methodology is based on the heterogeneous multiscale method (HMM). The HMM starts with an incomplete macroscopic model for macro variables on the macrogrid covering the full domain. The missing quantities and data in the macroscopic model are then obtained by solving an accurate microscale model locally over small domains. In the case at hand, the developed coupling method for the pressure equation uses local simulations on small sampled network domains at the pore scale to evaluate the continuum equation and thus solve for the pressure in the domain. The developed numerical algorithm for dynamic two-phase flows and its convergence are discussed in detail. The algorithm is given as a step-by-step procedure that is easy to implement for the interested reader. Computational experiments on both, single-phase flows with nonlinear flux-pressure dependence and the full two-phase flow, are presented.
- *Statistical geometry and topology applications in life sciences.* The use of concepts and methods of geometry, topology, and graph theory becomes increasingly important in life science applications. These applications include, but not limited to, the analysis of biological networks. A new method of characterizing tree networks based on structural triangulation of that network is developed in the present chapter by R.-K. Seong (Imperial, UK), P. Getreuer (Yale, USA), Y. Li, T. Girardi, C.M. Salafia (all Placental Analytics LLC, USA), and D.D. Vvedensky (Imperial, UK). A specific biological network is in the major focus in this chapter, namely the vasculature on the chorionic plate of a human placenta. For a graph-theoretical analysis, the vasculature is represented as edges and vertices. The developed method makes use of a triangulation of the tree network which enables one to formulate a partition function. Hence, the method can use then thermodynamic functions known from statistical mechanics as simple measures of the weighted topology of the corresponding tree network. The systematic variation of the introduced weights allows an examination of the development of the network. Several illustrative examples explaining the methodology and the algorithm behind are discussed. Finally, the developed methodology has been applied for the analysis of the arterial and venous vasculature of the chorionic plate of a variety of human placentas, and attempts have been made to examine the extent to which the entropy function is correlated to the infant birthweight with the sample set.
- *Optimal control applications with discrete and continuous features.* There is a wide range of applications where optimal control problems with discrete and continuous features arise naturally. This includes science and engineering, as well as

life science applications. A series of examples from such applications have been provided by S. Lenhart (University of Tennessee, USA), E. Bodine (Rhodes College, TN, USA), P. Zhong (Rutgers University, USA), and H.R. Joshi (Xavier University, OH, USA). Starting with several illustrative examples for optimal control with ordinary differential equations, the authors have explained in detail how the bang-bang and singular controls can be handled. Their examples include robotics applications where a mobile robot with one or more steerable drive wheels that steer together is considered. An example from population biology models species augmentation where two populations of the same species are described with a target endangered population and a reserve population. When the underlying systems are described by ODEs, problems which are linear in the control and have discrete values for the optimal control are emphasized. An extension to integro-difference models that are discrete in time and continuous in space is also given. This extension is illustrated with the optimal pest control problem where the underlying theory for characterization of an optimal control and necessary conditions are also discussed. Computational experiments for each of the examples described above complement the theory presented in this chapter. Details of numerical algorithms developed for such experiments are also given.

5 Concluding Remarks

An important pre-requisite of success of mathematical modeling and computational science as a driving force of scientific discovery and innovative, mathematics-based technologies is a closer collaboration of mathematicians with other disciplines. Only in this way, mathematical theories can evolve in a dynamic, sustainable manner as an essential part of human knowledge, and new mathematical models can stimulate new theoretical discoveries and new experimental findings.

At present, theoretical and experimental sciences, taken separately, are lacking systems-science-based approaches in studying phenomena, processes, and systems. Mathematical modeling and computational experiments can provide a missing link by complementing these two fundamental ways of human activities. They allow a two-way interaction between theory and natural experiment virtually in all areas where mathematical models can be constructed. They provide also a missing link in those cases where natural experiment is difficult or impossible to set up. This extends further the domain of mathematical modeling and mathematics-based technologies making them a decisive factor in sustainable socio-economic development and scientific-technological progress of our society.

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