

Computational Mathematics: An Application Prospective

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Abstract— Using concrete examples, we discuss the current and potential use of stochastic ordinary differential equations (SDEs) from the perspective of applied and computational mathematics. Assuming only a minimal background knowledge in probability and stochastic processes, we focus on aspects that distinguish SDEs from their deterministic counterparts. To illustrate a multiscale modelling framework, we explain how SDEs arise naturally as diffusion limits in the type of discrete-valued stochastic models used in chemical kinetics, population dynamics and, most typically, systems biology. We outline some key issues in existence, uniqueness and stability that arise when SDEs are used as physical models and point out possible pitfalls. We also discuss the use of numerical methods to simulate trajectories of an SDE and explain how both weak and strong convergence properties are relevant for highly efficient multilevel Monte Carlo simulations. We flag up what we believe to be key topics for future research, focussing especially on non-linear models, parameter estimation, uncertainty quantification, model comparison and multiscale simulation.

Keywords; *Computational Methods; Genetic Algorithms; Graph theory; Fractional Differential equations.*

I. INTRODUCTION

All Computational mathematics emerged as a distinct part of applied mathematics by the early 1950s. Much emphasis is given on using the computer as a tool to solve mathematically modeled physical problems. The result is a program or method that integrates mathematical theory into solutions for real-world problems, offering the best of both worlds: theoretical and computational mathematics. Computational Mathematics includes the study of problems that have applications in engineering, operations research medicine, and other areas of the sciences. These include many problems that affect our everyday life, from Internet security and telecommunication networking, to routes for school buses and delivery companies, scheduling tables,... etc. Researchers are recently applying computational

methods in many fields and it is difficult to summarize them in a few paragraphs, but the major themes of these works are applications in industry or technology. For example, construction of a new geomechanical quality, and applying machine learning techniques to the construction of these new geomechanical quality [4], and electricity production in hydroplants and building material [18]. There are also applications in surface science [25], laser crust removal [14], 3D models for energy and building [11].

There are also advances in medicine such as Illness-Death model, breast cancer diagnosis, acute sore throat diagnosis [7,16,19,8], and the treatment of medical problems on celestial bodies [12] that incorporate different algorithms and methods. There are also works where advances of mathematical and computational methods can be applied to other sciences and from these, industrial, or technological advances could be derived: from categorical algebra to formal context analysis [17], study of a variational inequality with a singular perturbation term [5]. Parallel mesh free computation for parabolic equations on graphics hardware [22]. Wavelet-based watermarking algorithms: theory, applications and critical aspects [2], and implementing a relational theorem prover for modal logic [20].

Bioinformatics is an emerging discipline that is rapidly growing up with the benefit of computer science and computational methods. In this sense, there many papers on the uses of evolutionary algorithms learning techniques to predict a determined health problem in humans [3], an improved feature reduction approach based on redundancy techniques for predicting female urinary incontinence [12], and another one that makes use of pattern analysis to handle database of leukemia patients [13]. Computational methods such as parallelization also contribute to the advancement of other disciplines. We can find three examples of this in the recent literature, namely improvements on binary coding using parallel computing [1], parallel mesh free computation for parabolic equations on graphics hardware [5], FASS: a hybrid parallel fast acoustic scattering solver [22]. Similarly, we can get significant improvements in theoretical disciplines from a computational point of view, such as in classification of mathematical objects; semifields [10], and Lie algebras [9].

Genetic Algorithms are used to generate useful solutions to optimization and search problems based on real life [15]. Genetic Algorithms are usually applied to spaces which are too large to be exhaustively searched, and they have many applications in bioinformatics, medical [19, 21, 24], economics, manufacturing, and in many other fields. Also, evolutionary fuzzy modeling has been applied to many

domains, branching into many areas as chemistry, telecommunications, biology, geophysics and medicine [3,6,23].

II. COMARA PARTICIPATING PAPERS

Our collection of papers in the special session Computational Mathematics in Real-life Applications, include three papers:

1- "Genetic Algorithm solution for the Doctor Scheduling Problem".

By Abir Alharbi, and Kholood Alqahtani from King Saud University, Saudi Arabia.

2- "Lyapunov's inequality for a fractional differential equation subject to a non-linear integral condition".

By Maysaa Al-Qurashi, and Lakhdar Ragoub. King Saud University, and Alyammama University.

3- "Graph Coloring applied to Medical Doctors Schedule" by Ferdous Tawfiq, and Kholood Alqahtani from King Saud University, Saudi Arabia.

The first paper entitled Genetic algorithms solution for Doctor Schedule problem, by Abir Alharbi and Kholood Alqahtani, proposes to solve the time schedule problem of doctors in a hospital using a computational method based on genetic evolution. In this study, a genetic algorithm solution to the scheduling problem for doctors in Pediatric Department is applied using a cost bit matrix of which each cell indicates any violation of constraints set by the hospital. The experimental results showed that the suggested method generated a doctor schedule faster and with less violated constraints compared to the traditional manual methods commonly used in hospitals.

The second paper entitled Lyapunov's inequality for fractional differential equation subject to a non-linear integral condition, by Maysaa Al-Qurashi and Lakhdar Ragoub, shows the non-existence of non-trivial solutions of appropriate eigenvalue fractional boundary value problem obeying an integral condition specified in the paper. The application of such conditions can be found in giving a bound for eigenvalues for which the eigenvalue problem has a nontrivial solution. The physical applications of eigenvalue problems are endless they appear in vibration analysis, quantum mechanics, environmental science. They are also used to model different types of population growth, financial equations, dynamic equations, stress and strain problems, and many more real life problems.

The third paper by Ferdous Tawfiq and Kholood Alqahtani presents a solution to the time schedule problem of doctors in a hospital using graph coloring theory. Graphs can be used to model many types of relations and processes in physical, biological, social, information systems, and many practical problems can be represented by graphs [24]. Proper coloring of a graph in the simplest form is an assignment of colors either to vertices of the graphs, or to its edges, in such a way that adjacent vertices/ edges are colored differently. The person performing Doctor

scheduling or Rota Organizer has to keep track of all the employees concerned, distributing hours fairly and avoiding collisions. The paper solved Doctors Scheduling Problem (DSP) and initialized a fair roster for two wards of the Pediatric Department by using the greedy algorithm from graph coloring theory.

III. CONCLUSION AND FUTURE WORK

Our special session COMARA: Computational Mathematics in Real-life Applications, have presented two papers using different computational methods that were applied to scheduling problem. Although it was presented for doctor scheduling, the results presented could be extended to other scheduling tables for routes, delivery, or student's time tables. Future research aims at experiments on the nurse's schedule in hospitals with more constraints and a diversity of requirements. Also, we propose to produce a software that helps hospitals design schedules with in their constraints for their doctors and nurses with simple inputs, less time and avoid conflicting manual schedules. Moreover, The Genetic algorithm and the Graph theory approaches to solving the doctor scheduling problem could be compared and analyzed in depth.

Considering all, we do believe that this collection of articles can be useful and informative on the new perspectives and trends in interactions between science, medicine, and engineering and hope that it can also serve as inspiration for new outcomes and other real life applications.

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